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Classical and Quantum Physics

60 Years Alberto Ibort Fest Geometry, Dynamics, and Control

Springer

Springer Proceedings in Physics

Volume 229

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Editors
G. Marmo
Università degli Studi di Napoli Federico II
Naples, Italy

David Martín de Diego
Institute of Mathematical Sciences (ICMAT)
Madrid, Spain

Miguel Muñoz Lecanda
Universitat Politècnica de Catalunya
Barcelona, Spain

ISSN 0930-8989 ISSN 1867-4941 (electronic)
Springer Proceedings in Physics
ISBN 978-3-030-24747-8 ISBN 978-3-030-24748-5 (eBook)
https://doi.org/10.1007/978-3-030-24748-5

This Springer imprint is published by the registered company Springer Nature Switzerland AG
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

Preface

This volume is dedicated to Alberto Ibort on his 60th birthday. Alberto has great and significantly contributed to many fields of mathematics and physics, always with highly original and innovative ideas.

Most of Albertos's scientific activity has been motivated by geometric ideas, concepts, and tools that are deeply related to the framework of classical dynamics and quantum mechanics. Let us mention some of the fields of expertise of Alberto Ibort: Geometric Mechanics; Constrained Systems; Variational Principles; Multisymplectic structures for field theories; Super-manifolds; Inverse problem for Bosonic and Fermionic systems; Quantum Groups, Integrable systems, BRST Symmetries; Implicit differential equations; Yang-Mills Theories; BiHamiltonian Systems; Topology Change and Quantum Boundary Conditions; Classical and Quantum Control; Orthogonal Polinomials; Quantum Field Theory and Noncommutative Spaces; Classical and Quantum Tomography; Quantum Mechanics on phase space; Wigner-Weyl formalism; Lie-Jordan Algebras, Classical and Quantum; Quantum-to-Classical transition; Contraction of Associative Algebras; contact geometry…

In each Alberto's contribution, one may find not only technical novelties but also completely new way of looking at the considered problems. Even an experienced reader, reading Alberto contributions on his field of expertise, will find new perspectives on the considered topic. His enthusiasm is happily contagious, for this reason he has had, and still has, very bright students wishing to elaborate their Ph.D. thesis under his guidance. What is more impressive, is the broad list of rather different topics on which he has contributed and the papers of this volume are just a sample.

It remains for us to wish that he will continue his creative scientific life for the next 60 years.

With our admiration

Naples, Italy — G. Marmo
Madrid, Spain — David Martín de Diego
Barcelona, Spain — Miguel Muñoz Lecanda

Alberto Ibort

Alberto Ibort was born in Huesca, on March 4, 1958. He received his education in Zaragoza, M.S. degrees in Physics and Mathematics and Ph.D. in Science (Physics) in 1984, from Universidad de Zaragoza, under the guidance of Prof. Jose F. Cariñena Marzo. After completion of his doctoral research, he was post-doc in Paris VI, Niels Bohr Institute and University of California at Berkeley in 1986 and 1990, before joining the Department of Física Teórica at University Complutense de Madrid, where he was Associate Professor until April 1997 when he won the chair of Applied Mathematics at the Department of Mathematics, Universidad Carlos III de Madrid.

He is member of the Real Sociedad Española de Física and Real Sociedad Matemática Española.

Ph.D. Students of Alberto Ibort Latre

1. **Jesús Marín Solano**. Fundamentos geométricos de Supermecánica Lagrangiana, Hamiltoniana y Supersimetría. Department of Theoretical Physics, Universidad Complutense de Madrid. Year 1992.
2. **Alejandro González Ruíz**. Modelos integrables bidimensionales con condiciones de contorno abiertas e invariancia bajo grupos cuánticos. Department of Theoretical Physics, Universidad Complutense de Madrid. Year 1993 (co-advised with H. de Vega).
3. **Fran Presas Mata**. Sobre la amplitud del fibrado precuantizable en geometría simpléctica y de contacto. Mathematics, Department of Álgebra, Universidad Complutense de Madrid Year 2000. Facultad de Matemáticas. Departamento de Álgebra, Universidad Complutense de Madrid (coadvised with I. Sols).
4. **David Martínez Torres**. Geometrías con caracter topológico. Departamento de Matemáticas, Universidad Carlos III de Madrid. Year 2003.
5. **Marina Delgado Téllez de Cepeda**. Métodos Geométricos en problemas de control óptimo singulares: fundamentos y aplicaciones. Departamento de Matemáticas, Universidad Carlos III de Madrid. Year 2004.
6. **Thalia Rodríguez de la Peña**. Reducción de principios variacionales con simetría y problemas de control óptimo de Lie-Scheers-Brockett. Departamento de Matemáticas, Universidad Carlos III de Madrid. Year 2009.
7. **Pablo Linares Briones**. Orthogonally additive polynomials and applications. Departamento de Análisis Matemático, Universidad Complutense de Madrid. Year 2009 (co-advised with J. L. G. Llavona).
8. **Juan Manuel Pérez-Pardo**. On the theory of self-adjoint extensions of the Laplace-Beltrami operator, quadratic forms and symmetry. Departamento de Matemáticas, Universidad Carlos III de Madrid. Year 2013 (co-advised with F. Lledo).
9. **Leonardo Ferro**. Symmetries and constraints in classical and quantum mechanics: Lie-Jordan Banach algebras and their applications. Departamento de Matemáticas, Universidad Carlos III de Madrid. Year 2013.
10. **Alberto López Yela**. Quantum Tomography: Foundations and applications. Departamento de Matemáticas, Universidad Carlos III de Madrid. Year 2015.
11. **Alfredo Bautista Santacruz**. On the causality properties of space-times, their spaces of light rays and skies. Departamento de Geometría y Topológia, Universidad Complutense de Madrid. Year 2016 (co-advised with J. Lafuente).

Master Students

1. **Juan Manuel Pérez-Pardo**. Master of Science (Física Teórica, UCM). Von Neumann Quantum Control. Departamento de Matemáticas, Universidad Carlos III de Madrid. Year 2009.
2. **Rafael Olano Libran**. Master of Science (Física Teórica, UCM). Quantum Algorithms for solving Linear Systems. Departamento de Fisica Teorica I, Universidad Complutense de Madrid. Year 2015.
3. **Aitor Balmaseda Martín**. Master of Mathematical Engineering (UC3M). Quantum Control at the Boundary: an application to Quantum Circuits. Year 2018.
4. **Nicolás de Miguel Ruano**. TFG, Industrial Technologies, UCIIIM Controlabilidad de sistemas híbridos. Escuela Politécnica Superior, Universidad Carlos III de Madrid. Year 2016.

List of Publications of Alberto Ibort

Books

J.F. Cariñena, A. Ibort, G. Marmo, G. Morandi. **Geometry from Dynamics, Classical and Quantum Theoretical, Mathematical and Computational Physics**, vol XXV. Springer (2014), 723 pages. ISBN: 978-94-017-9219-6 (Print).

Alberto Ibort and J. F. Cariñena

60 Years Alberto Ibort Fest Classical and Quantum Physics: Geometry, Dynamics and Control 5–9 March, 2018

Scientific Papers

1. J.F. Cariñena, L.A. Ibort. *Non-Noether constanst of motion.* J. Phys. A: Math. and Gen., 16, 1–7 (1983).
2. M. Asorey, J.F. Cariñena, L.A. Ibort. *Generalized canonical transformations for time dependent systems.* J. Math. Phys., 24, 2745–2750 (1983).
3. J.F. Cariñena, L.A. Ibort. *Lax equations arising from Lagrangian foliations.* Lett. Math. Phys., 8, 21–26 (1984).
4. J.F. Cariñena, L.A. Ibort. *Bilagrangian connections and the reduction of Lax equations.* Lett. Math. Phys., 8, 359–365 (1984).
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6. J.F. Cariñena, L.A. Ibort. *Locally Hamiltonian systems with symmety and a generalized Noether's theorem.* Il Nuovo Cim., 87B, 41–49 (1985).
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10. F. Cantrijn, J.F. Cariñena, M. Crampin, L.A. Ibort. *Reduction of degenerate Lagrangians.* J. Geometry and Physics, 3, 353–400 (1986).
11. M. Crampin, L.A. Ibort. *Graded Lie algebras of derivations and Ehresmann connections.* J. Math. Pures et Appl., 66, 113–125 (1987).
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Contents

Contributors

Filiberto Ares Departamento de Física Teórica, Universidad de Zaragoza and Centro de Astropartículas y Física de Altas Energías (CAPA), Zaragoza, Spain; International Institute of Physics, UFRN, Natal, RN, Brazil

Manuel Asorey Centro de Astropartículas y Física de Altas Energías, Departamento de Física Teórica, Universidad de Zaragoza, Zaragoza, Spain

A. P. Balachandran Department of Physics, Syracuse University, Syracuse, NY, USA

A. Balmaseda Depto. de Matemáticas, Universidad Carlos III de Madrid, Madrid, Leganés, Spain

José F. Cariñena Departamento de Física Teórica and IUMA, Facultad de Ciencias, Universidad de Zaragoza, Zaragoza, Spain

Dariusz Chruściński Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Toruń, Poland

F. M. Ciaglia Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany

Jesús Clemente-Gallardo Department of Theoretical Physics, Faculty of Sciences, University of Zaragoza, Zaragoza, Spain;
IUI BIFI, University of Zaragoza, Zaragoza, Spain

Javier de Lucas Department of Mathematical Methods in Physics, University of Warsaw, Warszawa, Poland

A. R. de Queiroz Instituto de Física, Universidade de Brasília, Brasilia, DF, Brazil

José G. Esteve Departamento de Física Teórica, Centro de Astropartículas y Física de Altas Energías (CAPA) and Instituto de Biocomputación y Física de Sistemas Complejos, Universidad de Zaragoza, Zaragoza, Spain

Fernando Falceto Departamento de Física Teórica, Centro de Astropartículas y Física de Altas Energías (CAPA) and Instituto de Biocomputación y Física de Sistemas Complejos, Universidad de Zaragoza, Zaragoza, Spain

Eduardo Fernández Universidad Complutense de Madrid, Facultad de Matemáticas, Madrid, Spain;
Instituto de Ciencias Matemáticas CSIC-UAM-UC3M-UCM, Madrid, Spain

F. Finkel Departamento de Física Teórica, Universidad Complutense de Madrid, Madrid, Spain

Antonio G. García Department of Mathematics, Universidad Carlos III de Madrid, Leganés-Madrid, Spain

A. González-López Departamento de Física Teórica, Universidad Complutense de Madrid, Madrid, Spain

José M. Gracia-Bondía Escuela de Física, Universidad de Costa Rica, San José, Costa Rica;
Departamento de Física Teórica, Universidad de Zaragoza, Zaragoza, Spain

Miguel A. Hernández-Medina Departamento de Matemática Aplicada a las Tecnologías de la Información y las Comunicaciones, E.T.S.I.T., U.P.M., Madrid, Spain

Alberto Ibort ICMAT and Department of Mathematics, Universidad Carlos III de Madrid, Leganés-Madrid, Spain

Jorge A. Jover-Galtier Centro Universitario de la Defensa de Zaragoza, Zaragoza, Spain

I. León Departamento de Física Teórica, Universidad Complutense de Madrid, Madrid, Spain

Fedele Lizzi INFN, Sezione di Napoli & Dipartimento di Fisica "E. Pancini", Università di Napoli Federico II, Napoli, Italy;
Departament de Física Quàntica i Astrofísica and Institut de Cíencies del Cosmos (ICCUB), Universitat de Barcelona, Barcelona, Spain

Fernando Lledó Department of Mathematics, University Carlos III Madrid, Leganés, Madrid, Spain;
Instituto de Ciencias Matemáticas (ICMAT), Madrid, Spain

F. Magri Dipartimento di Matematica ed Applicazioni, Università di Milano Bicocca, Milan, Italy

Margarita A. Man'ko Lebedev Physical Institute, Russian Academy of Sciences, Moscow, Russia

Vladimir I. Man'ko Lebedev Physical Institute, Russian Academy of Sciences, Moscow, Russia

G. Marmo Dipartimento di Fisica "E. Pancini", Università di Napoli Federico II, Complesso Universitario di Monte S. Angelo Edificio 6, via Cintia, Napoli, Italy

Juan Carlos Marrero Unidad asociada ULL-CSIC, Geometría Diferencial y Mecánica Geométrica Departamento de Matemática, Estadística e I.O., Universidad de la Laguna, Tenerife, Canary Islands, Spain

T. Marsico Liceo Classico Berchet, Milan, Italy

Diego Martínez Department of Mathematics, University Carlos III Madrid, Leganés, Madrid, Spain;
Instituto de Ciencias Matemáticas (ICMAT), Madrid, Spain

Javier Martínez-Aguinaga Universidad Complutense de Madrid, Facultad de Matemáticas, Madrid, Spain;
Instituto de Ciencias Matemáticas CSIC-UAM-UC3M-UCM, Madrid, Spain

Edith Padrón Unidad asociada ULL-CSIC, Geometría Diferencial y Mecánica Geométrica Departamento de Matemática, Estadística e I.O., Universidad de la Laguna, Tenerife, Canary Islands, Spain

J. M. Pérez-Pardo Depto. de Matemáticas, Universidad Carlos III de Madrid, Madrid, Leganés, Spain;
Instituto de Ciencias Matemáticas CSIC - UAM - UC3M - UCM (ICMAT), Madrid, Spain

Alexandr Pinzul Universidade de Brasília Instituto de Física & International Center of Physics, Brasilia, DF, Brazil

Francisco Presas Instituto de Ciencias Matemáticas CSIC-UAM-UC3M-UCM, Madrid, Spain

Manuel F. Rañada Departamento de Física Teórica and IUMA, Facultad de Ciencias, Universidad de Zaragoza, Zaragoza, Spain

A. F. Reyes-Lega Departamento de Física, Universidad de los Andes, Bogotá, Colombia

M. A. Rodríguez Departamento de Física Teórica, Universidad Complutense de Madrid, Madrid, Spain

Narciso Román-Roy Department of Mathematics, Barcelona, Spain

Alberto Saa Department of Applied Mathematics, University of Campinas, Campinas, SP, Brazil

Mariano Santander Departamento de Física Teórica and IMUVa, Facultad de Ciencias, Universidad de Valladolid, Valladolid, Spain

L. Schiavone Department of Mathematics, Faculty of Science, University of Ostrava, Ostrava, Czech Republic

Joseph C. Várilly Escuela de Matemática, Universidad de Costa Rica, San José, Costa Rica

Patrizia Vitale Dipartimento di Fisica "E. Pancini", Università di Napoli Federico II and INFN-Sezione di Napoli, Napoli, Italy

Chapter 1
On a New Asymptotic Behaviour of Toeplitz Determinants

Filiberto Ares, José G. Esteve and Fernando Falceto

Abstract In this paper we shall study the asymptotics of the logarithm of Toeplitz determinants whose symbol is intermediate between those that provide a finite asymptotic limit to the determinant and those that induce a linear growth with the logarithm of the dimension. We conjecture that in the intermediate case a new behaviour emerges in which the logarithm of the determinant diverges at a rate smaller than the logarithm of the dimension. We give the precise form of this asymptotic behaviour and support it with analytic and numerical arguments. We believe this is the first time that the intermediate regime is considered, as we were not able to find any reference to it in the literature.

1.1 Introduction

The History of the Toeplitz determinants is a very interesting example of the cross-breeding between Physics and Mathematics (see [1] for an excellent review). Of course, there is a vast literature on the subject and we will present below a very partial and biased account. In particular, we will focus on some conjectures, that later on became theorems, and will be important to support our results.

F. Ares
Departamento de Física Teórica, Universidad de Zaragoza and Centro de Astropartículas y Física de Altas Energías (CAPA), 50009 Zaragoza, Spain
e-mail: ares@unizar.es

International Institute of Physics, UFRN, Natal, RN 59078-970, Brazil

J. G. Esteve · F. Falceto (✉)
Departamento de Física Teórica, Centro de Astropartículas y Física de Altas Energías (CAPA) and Instituto de Biocomputación y Física de Sistemas Complejos,
Universidad de Zaragoza, 50009 Zaragoza, Spain
e-mail: falceto@unizar.es

J. G. Esteve
e-mail: esteve@unizar.es

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_1

Toeplitz operators are named after Otto Toeplitz who introduced them around 1907 as particular examples of the abstract theory that Hilbert was developing at that time.

Our focus will be on the behaviour of the determinant of these operators, i.e. Toeplitz determinants, when the dimension grows to infinity. The first result in this direction is due to Szegő [2] that in 1915 proved a conjecture by Polyia. The latter wrote the following comment in [3]

> Our cooperation started from a conjecture which I found. It was about a determinant considered by Toeplitz and others, formed with the Fourier coefficients of a function $f(x)$. I had no proof, but I published the conjecture and the young Szegő found the proof…

This is sometimes called *First Szegő theorem* and we will review it in the next section.

Almost 40 years later, Toeplitz determinants were shown to be crucial for solving problems of statistical physics. Namely, Kaufman and Onsager [4] found in 1949 that the magnetization of the Ising model in two dimensions below critical temperature could be obtained from the computation of a particular Toeplitz determinant. The problem was that Szegő's theorem on the asymptotic limit of the determinant gave a trivial result in this case, and the answer was in the next to leading correction which was not determined by the theorem.

Onsager, using an alternative form of computing the magnetization (that they did not publish), arrived at a conjecture for the form of the next to leading corrections for Toeplitz determinants. As he admitted, he was working to prove the conjecture, but at some point Szegő (again Szegő) was aware of Kaufman and Onsager's interest and in 1952 came out with the expression for the subleading corrections establishing the *Strong Szegő theorem* or *Second Szegő theorem* [5]. At this point it is interesting to recall Onsager's words quoted from [6]

> …and lo and behold I found it. It was a general formula for the evaluation of Toeplitz matrices. The only thing I did not know was how to fill out the holes in the mathematics and show the epsilons and deltas and all that…
>
> …the mathematicians got there first…

The third conjecture that we will review is also related to the Ising model and provides the asymptotic expansion of the Toeplitz determinant for symbols with zeros or discontinuities. This case is not considered in the Second Szegő Theorem but has a great physical interest: for instance, from this result one can derive the correlation function for the critical Ising model.

Fisher and Hartwig in 1968 [7], using partial results due to the physicists Lenard [8] and Wu [9] together with further insights, arrived at an expression for Toeplitz determinants for symbols that include zeros or discontinuities. The proof of this conjecture is due to Widom (1972) [10], when discontinuities are absent, and Basor (1978) [11], in full generality. Later on, it was discovered that in some cases the Fisher-Hartwig conjecture do not apply. Basor and Tracy understood the reason for this anomaly and conjectured the correct expression for the determinant in [12]. It was finally proven to be right by Deift et al. [13].

In this paper we want to present and motivate another conjecture on the Toeplitz determinant for symbols that, even if they are continuous, do not fulfill the requirements of the Second Szegő Theorem. We will give strong evidences and analytical arguments to show that the determinant has an asymptotic behaviour which is different from those considered previously in the literature. Finally, we will briefly discuss the possible physical implications of our result.

1.2 The Two Szegő's Theorems

Consider an integrable complex function defined on the unit circle $f : S^1 \to \mathbb{C}$. We shall denote by $T_N[f]$ the Toeplitz matrix with symbol f and dimension $N \times N$. Its entries $(T_N[f])_{nm} = f_{n-m}$ are given by the Fourier coefficients of the function f,

$$f_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(\theta)\mathrm{e}^{\mathrm{i}\theta k}\mathrm{d}\theta.$$

Let us also introduce the Fourier coefficients of $\log f$,

$$s_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} \log f(\theta)\mathrm{e}^{\mathrm{i}\theta k}\mathrm{d}\theta.$$

Assume that f is real and positive, then the **(First) Szegő theorem** [2] establishes that the dominant term of its determinant $D_N[f] = \det T_N[f]$ should be

$$\log D_N[f] = Ns_0 + o(N). \tag{1.1}$$

Observe that this theorem does not say anything about the correction $o(N)$. But, as it was recognized by Szegő, it happens to be finite if the symbol f is *smooth enough*[1] such that

$$\sum_{k=-\infty}^{\infty} |f_k| + \sum_{k=-\infty}^{\infty} |k||f_k|^2 < \infty. \tag{1.2}$$

In this case, the **Strong Szegő theorem** states that the correction in (1.1) is finite in the limit $N \to \infty$ [5, 14],

$$\log D_N[f] = Ns_0 + \sum_{k=1}^{\infty} ks_k s_{-k} + o(1). \tag{1.3}$$

The series in the expression above diverges when, for example, the symbol f has a jump discontinuity. In this case the **Fisher-Hartwig conjecture** [7, 11] precisely

[1] This is the case if the symbol is $C^{1+\varepsilon}$, i.e. its derivative is Hölder continuous with exponent $\varepsilon > 0$.

gives the next terms in $o(N)$. If the symbol f presents discontinuities at $\theta_1, \ldots, \theta_R$, the next term in the expansion (1.1) is logarithmic,

$$\log D_N[f] = Ns_0 + \frac{\log N}{4\pi^2} \sum_{r=1}^{R} \left(\log \frac{f_r^-}{f_r^+} \right)^2 + \log E[f] + o(1), \tag{1.4}$$

where $f_r^{\pm}$ are the lateral limits of f at the discontinuity point θ_r,

$$f_r^+ = \lim_{\theta \to \theta_r^+} f(\theta) \quad \text{and} \quad f_r^- = \lim_{\theta \to \theta_r^-} f(\theta),$$

and $\log E[f]$ a constant term.

1.3 The Fisher-Hartwig Conjecture Revisited

In this Section we shall see how Fisher and Hartwig arrived at their result, extending somehow the domain of applicability of the Strong Szegő Theorem (SST). This will allow us to establish a more general conjecture for the asymptotic behaviour of Toeplitz determinants with a continuous symbol that, however, does not satisfy the smoothness condition of the SST.

In the original formulation of the SST [5], Szegő considered that the symbol f must have a derivative satisfying the Hölder continuity condition for a non-zero exponent. In the following years, many mathematicians tried to weak this assumption. There is a plethora of papers were the SST is proved using different methods and considering more general symbols, see for instance the works by Kac [15], Baxter [16], Ibraginov [14] or Hirschman [17]. When we enunciated the SST in the previous section, we considered the smoothness condition (1.2) due to Hirschman. This is in some sense the weakest condition for the smoothness of the symbol f. As Devinatz showed in [18], for a real symbol such that $0 < f(\theta) < \infty$

$$\lim_{N \to \infty} \frac{D_N[f]}{\mathrm{e}^{Ns_0}} = \mathrm{e}^{\sum_{k=1}^{\infty} k s_k s_{-k}} < \infty$$

if an only if f verifies (1.2).

For simplicity, and as Fisher and Hartwig precisely did, we take the symbol

$$f_0(\theta) = \mathrm{e}^{\beta(\theta - \pi \operatorname{sign}(\theta))}, \quad \theta \in [-\pi, \pi), \tag{1.5}$$

that only has a discontinuity at $\theta = 0$.

The Fourier coefficients of its logarithm are

$$s_0^{(0)} = 0, \quad \text{and} \quad s_k^{(0)} = \frac{\beta}{\mathrm{i}k}, \quad \text{for} \quad k \neq 0.$$

Then if we apply to this symbol the Strong Szegő Theorem (1.3) we obtain the Harmonic series

$$\log D_N[f_0] = N s_0^{(0)} + \sum_{k=1}^{\infty} k s_k^{(0)} s_{-k}^{(0)} + o(1) = \sum_{k=1}^{\infty} \frac{\beta^2}{k} + o(1),$$

that diverges logarithmically.

Let us suppose that $\log D_N[f_0]$ can be obtained truncating the series $\sum_{k=1}^{\infty} k s_k^{(0)} s_{-k}^{(0)}$ at some $k = \lfloor N\Lambda_0 \rfloor$, with Λ_0 a positive real number. Here $\lfloor t \rfloor$ means to take the integer part of the real number t. Then we find

$$\log D_N[f_0] = \sum_{k=1}^{\lfloor N\Lambda_0 \rfloor} k s_k^{(0)} s_{-k}^{(0)} = \sum_{k=1}^{\lfloor N\Lambda_0 \rfloor} \frac{\beta^2}{k} = \beta^2 \log(N\Lambda_0) + \beta^2 \gamma_{\mathrm{E}} + o(1), \quad (1.6)$$

where γ_{E} is the Euler-Mascheroni constant.

Observe that this truncation precisely gives the Fisher-Hartwig expansion (1.4) for the symbol f_0. In fact, since $f_0(\theta)$ presents a single discontinuity ($R = 1$) with lateral limits $\mathrm{e}^{\pm\beta\pi}$, the expression in (1.4) particularizes to

$$\log D_N[f_0] = \beta^2 \log N + \log E[f_0] + o(1). \quad (1.7)$$

Comparing (1.7) with (1.6) we can conclude that

$$\log E[f_0] = \beta^2(\log \Lambda_0 + \gamma_{\mathrm{E}}). \quad (1.8)$$

Fisher and Hartwig were able to fix the constant term $E[f_0]$ and, therefore, the cutoff parameter Λ_0 because they realized that the Toeplitz matrix with symbol f_0 is also a Cauchy matrix.[2] Using the properties of the determinants of Cauchy matrices they determined that

$$E[f_0] = G(1 + \mathrm{i}\beta)G(1 - \mathrm{i}\beta)$$

where $G(z)$ is the Barnes G-function. Hence we have

$$\log \Lambda_0 = 2\beta^{-2} \log |G(1 + \mathrm{i}\beta)| - \gamma_{\mathrm{E}}. \quad (1.9)$$

The same reasoning can be applied to a general symbol with R discontinuities. The asymptotic behaviour of its determinant predicted by (1.4) can be deduced from the Strong Szegő theorem (1.3) truncating the divergent terms in the series $\sum_{k=1}^{\infty} k s_k s_{-k}$.

The previous discussion suggests that one could deduce heuristically from the Strong Szegő Theorem the asymptotic behaviour of a Toeplitz determinant generated by a symbol that violates the smoothness condition (1.2). When this happens the series

[2] A matrix is of Cauchy type if its entries are of the form $C_{nm} = (X_n - Y_m)^{-1}$ with $X_n - Y_m \neq 0$, and $X_n, Y_m \in \mathbb{C}$ where $n, m \in \mathbb{N}$.

in (1.3) diverges. We propose that the truncation of this series at $k = \lfloor N\Lambda \rfloor$, with Λ certain positive real number, accounts for the asymptotic expansion of the Toeplitz determinant. That is, if the symbol f is not smooth enough, then the corresponding determinant behaves as

$$\log D_N[f] = Ns_0 + \sum_{k=1}^{\lfloor N\Lambda \rfloor} k s_k s_{-k} + o(1).$$

In the next section we shall check this conjecture for a family of continuous symbols that does not satisfy the smoothness condition of the Strong Szegő Theorem.

1.4 Generalization of the Fisher-Hartwig Conjecture

Consider the symbols of the form

$$\log g_\nu(\theta) = \beta \frac{\theta - \pi \operatorname{sign}(\theta)}{\left(-\log \frac{|\theta|}{2\pi}\right)^\nu}, \quad \theta \in [-\pi, \pi), \tag{1.10}$$

with $\beta < 1$ and $\nu \geq 0$.

In Fig. 1.1 we plot $\log g_\nu(\theta)$ for $\beta = 1/\pi$ and different values of ν. It is a family of positive bounded functions, $0 < g_\nu(\theta) < \infty$. For $\nu \neq 0$ the function is continuous but it is non analytical at $\theta = 0$ since its derivative diverges at this point. For $\nu = 0$,

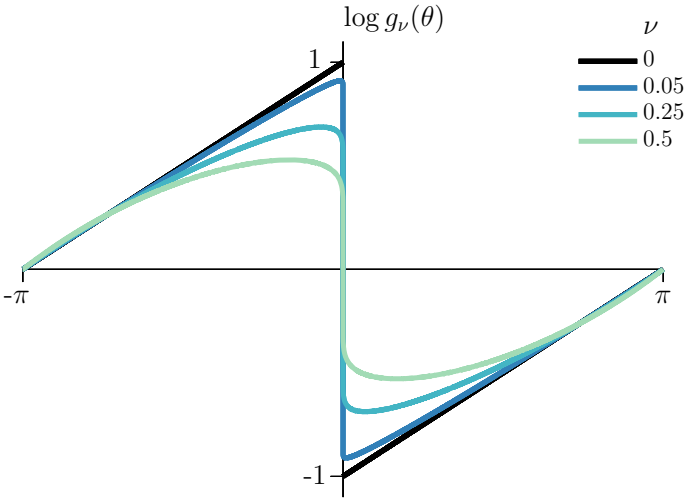

Fig. 1.1 Plot of the logarithm of the symbol g_ν defined in (1.10), taking $\beta = 1/\pi$ and different values for the exponent ν. If $\nu = 0$ the function $g_0(\theta)$ is discontinuous at $\theta = 0$. When $\nu > 0$ the symbol is continuous for all θ but its derivative diverges at $\theta = 0$

it reduces to the symbol (1.5), studied in the previous section, that has a discontinuity at $\theta = 0$. Then in this limiting case the Fisher-Hartwig conjecture can be applied.

According to the discussion in the previous section, in order to determine the asymptotic behaviour of the Toeplitz determinant generated by g_ν, we have to study the convergence of the series

$$\sum_{k=1}^{\infty} k s_k^{(\nu)} s_{-k}^{(\nu)}, \tag{1.11}$$

where $s_k^{(\nu)}$ are the Fourier coefficients of $\log g_\nu$,

$$s_k^{(\nu)} = \frac{1}{2\pi} \int_{-\pi}^{\pi} \log g_\nu(\theta) \mathrm{e}^{\mathrm{i}k\theta} \mathrm{d}\theta.$$

If we compute the asymptotic expansion of $s_k^{(\nu)}$ up to first order corrections we obtain

$$s_k^{(\nu)} \sim -\frac{\mathrm{i}\beta}{k(\log|k|)^\nu} + \frac{\mathrm{i}\beta\nu(\log(2\pi) + \gamma_{\mathrm{E}})}{k(\log|k|)^{\nu+1}} + O\left(\frac{1}{k(\log|k|)^{\nu+2}}\right). \tag{1.12}$$

Therefore, the series (1.11) converges if and only if

$$\sum_{k=2}^{\infty} \frac{\beta^2}{k(\log k)^{2\nu}} < \infty.$$

Using for instance the integral test it is immediate to see that the latter diverges for $0 \leq \nu \leq 1/2$. Thus for these values of the exponent ν the Strong Szegő theorem (1.3) is not valid to determine the asymptotic behaviour of $D_N[g_\nu]$. We emphasize again that for $\nu \neq 0$ the function is continuous and we can neither employ the Fisher-Hartwig conjecture that only applies to symbols with discontinuities and/or zeros.

Therefore, we have to resort to the conjecture that we have proposed at the end of the previous section. We conjecture that there exists a positive and real number Λ_ν, that depends on ν, such that the asymptotic behaviour of the Toeplitz determinant with symbol g_ν is given by

$$\log D_N[g_\nu] = N s_0^{(\nu)} + \sum_{k=1}^{\lfloor N\Lambda_\nu \rfloor} k s_k^{(\nu)} s_{-k}^{(\nu)} + o(1).$$

Since $\log g_\nu(\theta)$ is an odd function then $s_{-k}^{(\nu)} = -s_k^{(\nu)}$. Hence $s_0^{(\nu)} = 0$, the linear term in $\log D_N[g_\nu]$ cancels, and

$$\log D_N[g_\nu] = \sum_{k=1}^{\lfloor N\Lambda_\nu \rfloor} k|s_k^{(\nu)}|^2 + o(1). \tag{1.13}$$

This conjecture predicts a sublogarithmic growth of $\log D_N[g_\nu]$ with the dimension N. In fact, if we consider the asymptotic behaviour (1.12) found for $s_k^{(\nu)}$ and we approximate the sum in (1.13) by an integral,

$$\sum_{k=1}^{\lfloor N\Lambda_\nu \rfloor} k|s_k^{(\nu)}|^2 \sim \int_{1+\varepsilon}^{N\Lambda_\nu} \frac{\beta^2}{\theta(\log\theta)^{2\nu}} \left[1 + O\left(\frac{1}{\log\theta}\right)\right] \mathrm{d}\theta \tag{1.14}$$

where $\varepsilon > 0$. The error that it is made approximating the sum by the integral is of the order of $N^{-1}(\log N)^{-2\nu}$.

Therefore, for $0 < \nu < 1/2$ we have

$$\sum_{k=1}^{\lfloor N\Lambda_\nu \rfloor} k|s_k^{(\nu)}|^2 \sim \frac{\beta^2}{1-2\nu}(\log N\Lambda_\nu)^{1-2\nu} + O\left(\frac{1}{(\log N)^{2\nu}}\right).$$

Observe that the contribution of the subleading terms in the asymptotic behaviour (1.12) of the Fourier coefficients $s_k^{(\nu)}$ tends to zero in the limit $N \to \infty$.

If we take into account that

$$(\log N\Lambda_\nu)^{1-2\nu} = (\log N)^{1-2\nu}\left(1 + \frac{\log\Lambda_\nu}{\log N}\right)^{1-2\nu},$$

and employ the expansion $(1+z)^a = 1 + az + O(z^2)$ for $z < 1$ and $a > 0$, we find

$$\sum_{k=1}^{\lfloor N\Lambda_\nu \rfloor} k|s_k^{(\nu)}|^2 \sim \frac{\beta^2}{1-2\nu}(\log N)^{1-2\nu} + o(1), \quad \text{if } 0 < \nu < 1/2.$$

On the other hand, for $\nu = 1/2$, the approximation in (1.14) leads to

$$\sum_{k=1}^{\lfloor N\Lambda_\nu \rfloor} k|s_k^{(\nu)}|^2 \sim \beta^2 \log\log N\Lambda_\nu + O\left(\frac{1}{\log N}\right).$$

Expressing the latter as

$$\log\log(N\Lambda_\nu) = \log\log N + \log\left(1 + \frac{\log\Lambda_\nu}{\log N}\right),$$

and applying the expansion $\log(1+z) = z + O(z^2)$ when $z < 1$, then

$$\sum_{k=1}^{\lfloor N\Lambda_\nu \rfloor} k|s_k^{(\nu)}|^2 \sim \beta^2 \log\log N + o(1).$$

Finally, putting these results in the conjecture (1.13) we can conclude that

$$\log D_N[g_\nu] = \frac{\beta^2}{1-2\nu}(\log N)^{1-2\nu} + o(1), \quad \text{if } 0 < \nu < 1/2,$$

and

$$\log D_N[g_{1/2}] = \beta^2 \log\log N + o(1), \quad \text{if } \nu = 1/2.$$

Observe that for $\nu = 0$ the conjecture (1.13) gives the Fisher-Hartwig expansion (1.6) with Λ_0 that given in (1.9).

Let us check (1.13) numerically. Since $\log D_N[g_\nu]$ grows sublogarithmically with the dimension N, we have to calculate it for a large range of N. In fact, notice that $(\log 100)^{0.25} = 1.46491\ldots$ and, if we increase N two orders of magnitude, $(\log 10,000)^{0.25} = 1.74208\ldots$. The problem is that if we go to larger values of N, we must diagonalize matrices of dimensions that are impossible to cope with a standard computer.

In principle, since the entries of a Toeplitz matrix only depend on the difference between the row and the column, the complete matrix is determined specifying a single row or column. However, we do not know any specific routine for computing Toeplitz determinants that makes use of this property. Hence it is needed to store the N^2 complex entries to calculate the determinant. If we work in double precision in C, each entry typically occupies 8 bytes of RAM memory. Thus, making a crude estimate, if the dimension of the matrix is N=20,000, we will need around 6 GB of memory, and if we take N=50,000, the amount of memory required increases to 37 GB.

We have bypassed that difficulty performing the numerical calculations in the supercomputer *Memento*, managed by the Instituto de Biocomputación and Física de Sistemas Complejos, that it is part of the University of Zaragoza. Each node of this cluster has 256 GB of memory. This has allowed us to reach dimensions of the order of $N = 10^5$. We have computed $\log D_N[g_\nu]$ from the spectrum of the matrix that has been obtained using the routines for Hermitian matrices provided in the Intel MKL library [19]. This library allows to parallelize the diagonalization, taking advantage of the 64 cores available in each node of *Memento*.

In Fig. 1.2, the dots represent the numerical values calculated with *Memento* for $\log D_N[g_\nu]$ with $\nu = 0, 0.05, 0.25$, and 0.50. The dashed lines represent the sum

$$\sum_{k=1}^{N} k|s_k^{(\nu)}|^2, \tag{1.15}$$

that is, assuming $\Lambda_\nu = 1$. The Fourier coefficients $s_k^{(\nu)}$ have been computed numerically for each ν. Comparing the dashed lines with the numerical points it is clear the necessity of considering a cutoff Λ_ν different from the unity. We have estimated its value for each ν as follows.

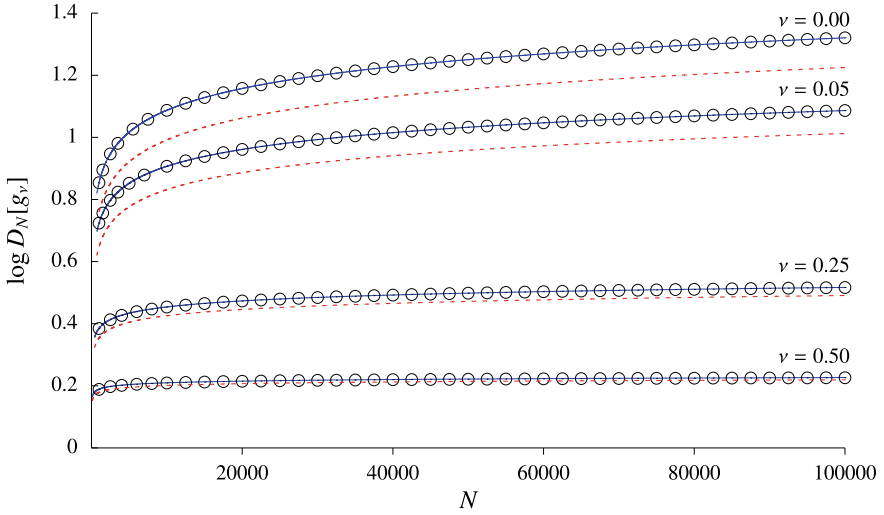

Fig. 1.2 Logarithm of the Toeplitz determinant with symbol the function g_ν defined in (1.10). We represent it against the dimension N. The dots correspond to the numerical values obtained using *Memento* for different exponents ν and $\beta = 1/\pi$. When $0 \leq \nu \leq 1/2$, g_ν does not satisfy the smoothness condition (1.2) of the Strong Szegő Theorem. The solid lines represent the conjecture proposed in (1.13) for the asymptotic behaviour of $\log D_N[g_\nu]$, $\sum_{k=1}^{\lfloor N\Lambda_\nu \rfloor} k|s_k^{(\nu)}|^2$, with Λ_ν those given in Table 1.1. For $\nu = 0$ the symbol is discontinuous and we can apply the Fisher-Hartwig conjecture. In this case Λ_0 can be directly calculated using (1.9). The dashed lines correspond to the sum $\sum_{k=1}^{N} k|s_k^{(\nu)}|^2$, that is considering $\Lambda_\nu = 1$

Consider the difference between taking $\Lambda_\nu = 1$ and $\Lambda_\nu > 1$,

$$\sum_{k=N}^{\lfloor N\Lambda_\nu \rfloor} k|s_k^{(\nu)}|^2.$$

For large N, if we take the asymptotic expansion (1.12) for $s_k^{(\nu)}$ and we approximate the sum by an integral, we have

$$\sum_{k=N}^{\lfloor N\Lambda_\nu \rfloor} k|s_k^{(\nu)}|^2 \sim \int_N^{N\Lambda_\nu} \left(\frac{\beta^2}{\theta(\log\theta)^{2\nu}} - \frac{2\nu\beta^2(\log(2\pi)+\gamma_{\mathrm{E}})}{\theta(\log\theta)^{2\nu+1}} \right) \mathrm{d}\theta.$$

The first term in the integral gives

$$\begin{aligned} \int_N^{N\Lambda_\nu} \frac{\beta^2}{\theta(\log\theta)^{2\nu}} \mathrm{d}\theta &= \frac{\beta^2}{1-2\nu}(\log N)^{1-2\nu} \left[\left(1 + \frac{\log\Lambda_\nu}{\log N} \right)^{1-2\nu} - 1 \right] \\ &= \frac{\beta^2 \log\Lambda_\nu}{(\log N)^{2\nu}} - \frac{\nu\beta^2(\log\Lambda_\nu)^2}{(\log N)^{2\nu+1}} + O\left((\log N)^{-2\nu-2} \right), \end{aligned}$$

where we have employed the expansion $(1+z)^{-a} = 1 - az - a(1-a)z^2/2 + O(z^3)$ for $z < 1$ and $a > 0$.

With respect to the second term in the integral, we follow the same lines

$$\int_N^{N\Lambda_\nu} \frac{2\nu\beta^2(\log(2\pi)+\gamma_{\mathrm{E}})}{\theta(\log\theta)^{2\nu+1}}\mathrm{d}\theta = -\beta^2(\log(2\pi)+\gamma_{\mathrm{E}})(\log N)^{-2\nu}\left[\left(1+\frac{\log\Lambda_\nu}{\log N}\right)^{-2\nu}-1\right]$$
$$= \frac{2\nu(\log(2\pi)+\gamma_{\mathrm{E}})\beta^2\log\Lambda_\nu}{(\log N)^{2\nu+1}} + O\left((\log N)^{-2\nu-2}\right).$$

Putting all together, we have

$$\sum_{k=N}^{\lfloor N\Lambda_\nu\rfloor} k|s_k^{(\nu)}|^2 \sim \frac{\beta^2\log\Lambda_\nu}{(\log N)^{2\nu}} - \frac{2\nu(\log(2\pi)+\gamma_{\mathrm{E}})\beta^2\log\Lambda_\nu + \nu\beta^2(\log\Lambda_\nu)^2}{(\log N)^{2\nu+1}}. \quad (1.16)$$

Therefore, a way to estimate Λ_ν is to calculate the difference between the numerical values obtained for $\log D_N[g_\nu]$ and the sum $\sum_{k=1}^N k s_k^{(\nu)} s_{-k}^{(\nu)}$ and use the result to fit the function in the right hand side of (1.16) where Λ_ν is the only parameter to be adjusted.

In order to perform the fit, we have considered the numerical values obtained in the interval $N \in [10^4, 10^5]$. Taking into account that $\beta = 1/\pi$, in Table 1.1 we indicate the values of Λ_ν that give the best fit.

The solid lines in Fig. 1.2 represent the sum $\sum_{k=1}^{\lfloor N\Lambda_\nu\rfloor} k|s_k^{(\nu)}|^2$ using the values for the cutoff Λ_ν collected in Table 1.1. The agreement between them and the numerical points is outstanding.

In Fig. 1.3, we represent separately the same results for each value of ν considered. In the inset of these figures we have plotted the difference between the numerical values obtained for the determinant and our prediction,

$$\Delta(N) = \log D_N[g_\nu] - \sum_{k=1}^{\lfloor N\Lambda_\nu\rfloor} k|s_k^{(\nu)}|^2. \quad (1.17)$$

Table 1.1 Values of Λ_ν for different ν and $\beta = 1/\pi$ obtained by fitting the curve on the right hand side of (1.16) to the difference between the numerical values computed for $\log D_N[g_\nu]$ and the sum $\sum_{k=1}^N k|s_k^{(\nu)}|^2$. The case $\nu = 0.00$ has been calculated using the expression (1.9)

ν	Λ_ν
0.00	2.566
0.05	2.599
0.25	2.659
0.50	2.660

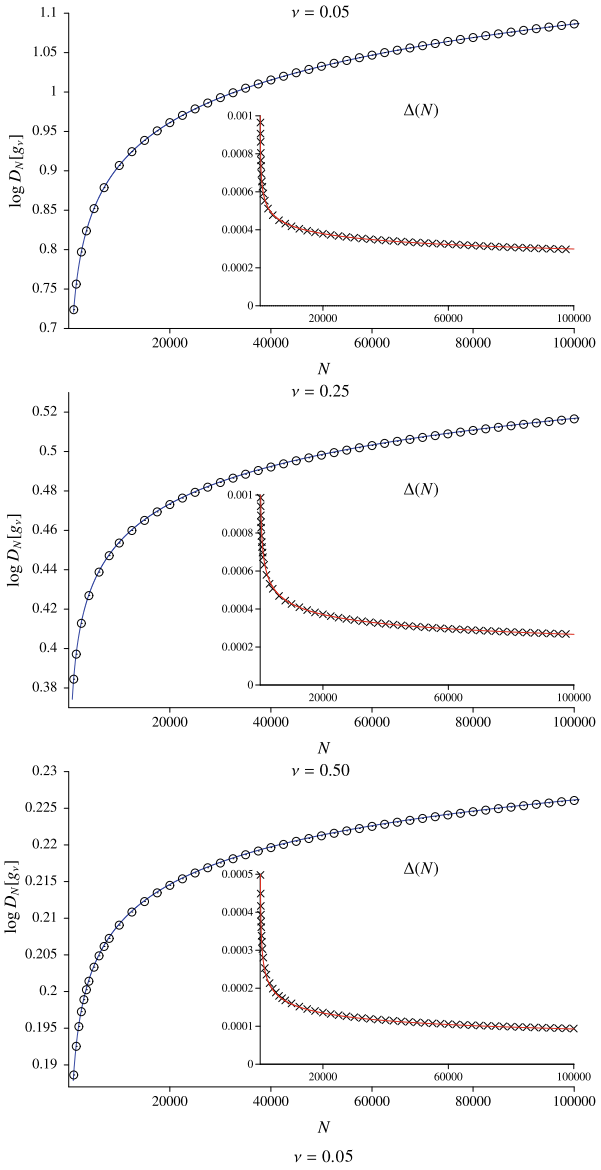

Fig. 1.3 Logarithm of the Toeplitz determinant generated by the symbol g_ν defined in (1.10) for $\beta = 1/\pi$, and $\nu = 0.05$ (up), 0.25 (middle) and 0.50 (bottom). The dots correspond to the numerical results obtained for the determinant varying the dimension N while the solid line represents the conjecture $\sum_{k=1}^{\lfloor N\Lambda_\nu \rfloor} k|s_k^{(\nu)}|^2$ using as Λ_ν the values given in Table 1.1. In the inset the crosses are the difference (1.17) between the numerical values and the prediction. The solid line in the inset corresponds to the curve a/N^b with the coefficients a and b those specified in Table 1.2. This curve is the best fit that we have found for $\Delta(N)$

Table 1.2 Coefficients a and b that give the best fit of the curve a/N^b to the difference between the outcomes in the numerical calculation of $\log D_N[g_\nu]$ and the conjectured behaviour $\sum_{k=1}^{\lfloor N\Lambda_\nu \rfloor} k|s_k^{(\nu)}|^2$ using for Λ_ν the values determined in Table 1.1

ν	a ($\times 10^{-3}$)	b
0.05	1.65	0.149
0.25	2.84	0.205
0.50	1.37	0.232

We have found that the best fit to this difference is the curve

$$\Delta(N) \approx \frac{a}{N^b},$$

with the value for the coefficients a and b indicated in Table 1.2.

1.5 Application to a Principal Submatrix

In the previous paper [20] we proposed and checked numerically a conjecture for the asymptotic behaviour of the determinant of a principal submatrix of a Toeplitz matrix. It is natural to ask whether those results are still valid in this context.

Consider the restriction of the Toeplitz matrix generated by g_ν to a subset of indices X, that we denote $T_X[g_\nu]$. For simplicity, let us assume that $X = [x_1, x_2] \cup [x_3, x_4]$. Then, according to the conjecture established in [20], the determinant $D(X) = \det T_X[g_\nu]$ should behave as

$$D\left([x_1, x_2] \cup [x_3, x_4]\right) \simeq \frac{D([x_1, x_4])D([x_1, x_2])D([x_2, x_3])D([x_3, x_4])}{D([x_1, x_3])D([x_2, x_4])} \tag{1.18}$$

where $\simeq$ stands for the equality of the asymptotic behaviour when $|x_\tau - x_{\tau'}| \to \infty$ for $\tau, \tau' = 1, \ldots, 4$.

The determinants on the right hand side of (1.18) correspond to Toeplitz matrices with symbol g_ν. Then we can apply to them the conjecture (1.13),

$$\log D([x_\tau, x_{\tau'}]) = \sum_{k=1}^{\lfloor N_{\tau,\tau'}\Lambda_\nu \rfloor} k|s_k^{(\nu)}|^2 + o(1), \tag{1.19}$$

where $N_{\tau,\tau'} = |x_\tau - x_{\tau'}|$.

In order to check the validity of the expression (1.18) we introduce the quantity

$$I_D\left([x_1, x_2] \cup [x_3, x_4]\right) = \log D([x_1, x_2]) + \log D([x_3, x_4]) - \log D\left([x_1, x_2] \cup [x_3, x_4]\right). \tag{1.20}$$

Applying (1.18), we have

$$I_D([x_1, x_2] \cup [x_3, x_4]) \simeq -\log \frac{D([x_1, x_4])D([x_2, x_3])}{D([x_1, x_3])D([x_2, x_4])}.$$

Considering now the expected asymptotic behaviour (1.19) for the Toeplitz determinants $D([x_\tau, x_{\tau'}])$, $\tau, \tau' = 1, \ldots, 4$, we arrive at

$$I_D\left([x_1, x_2] \cup [x_3, x_4]\right) \simeq \sum_{p,p'=1}^{2} (-1)^{p+p'} \sum_{k=1}^{\lfloor N_{p,p'+2} \Lambda_\nu \rfloor} k |s_k^{(\nu)}|^2. \tag{1.21}$$

In Fig. 1.4 we have evaluated numerically I_D for the exponents $\nu = 0.05$, 0.25 and 0.50 taking $\beta = 1/\pi$. The solid line corresponds to the prediction that we have just obtained in (1.21). In order to plot it, we have computed numerically the Fourier coefficients $s_k^{(\nu)}$ and we have assumed for Λ_ν the values estimated in Table 1.1. The agreement between the numerical outcome and the expected behaviour is extraordinary. This also reinforces the conjecture proposed for the Toeplitz determinants with symbol g_ν.

1.6 Conclusions

In this paper we have studied the large dimension behaviour for Toeplitz determinants with continuous symbols that do not lie within the application domain of the Strong Szegő theorem.

We propose a new asymptotic regime that leads to the sublogarithmic growth of the log-determinant. That is, the logarithm of the determinant of the Toeplitz matrix behaves like $(\log N)^\alpha$ for some $0 < \alpha < 1$, here N is the dimension. We also find a situation with a $\log \log N$ behaviour.

We should mention that this asymptotic regime for a Toeplitz determinant was not previously observed.

We support our conjecture with numerical simulations, finding a very good agreement that leaves little doubt about the correctness of our proposal.

Finally, we apply the results to a different related problem, that of the asymptotic behaviour of a principal submatrix of a Toeplitz matrix that we have studied in a previous publication. Again the agreement of our conjecture and the numerical simulation is excellent.

As a possible physical application of these ideas we mention the entanglement entropy in the Kitaev chain with long range couplings, whose Hamiltonian is

$$H = \sum_{n=1}^{N} \left(h a_n^\dagger a_n + a_n^\dagger a_{n+1} + a_{n+1}^\dagger a_n \right) + \sum_{n=1}^{N} \sum_{l=1}^{N/2} \frac{2}{l(\log(Al))^\nu} \left(a_n^\dagger a_{n+l}^\dagger - a_n a_{n+l} \right),$$

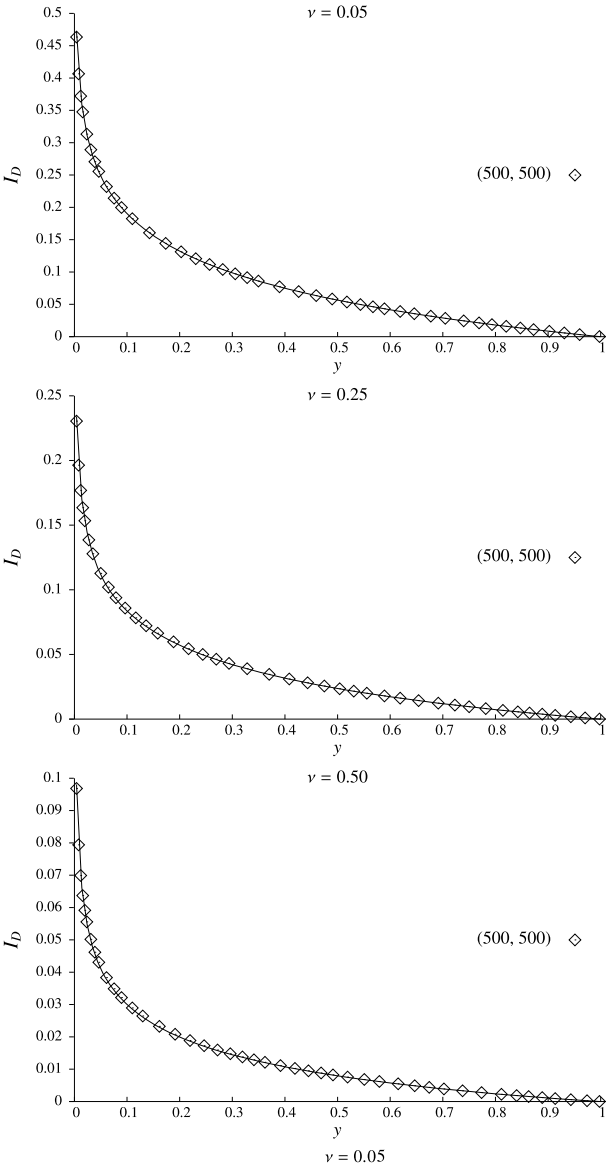

Fig. 1.4 Difference between the determinants (1.20) for the symbol g_ν defined in (1.10) considering $\beta = 1/\pi$ and $\nu = 0.05$ (up), 0.25 (middle) and 0.5 (bottom). We represent it as a function of the cross-ratio $y = \frac{(x_3-x_2)(x_4-x_1)}{(x_3-x_1)(x_4-x_2)}$. In all the cases we have taken $|x_1 - x_2| = |x_3 - x_4| = 500$ and we have modified the distance $|x_2 - x_3|$ from 1 up to 10,000. The dots $\diamond$ are the results of the numerical calculations while the solid line corresponds to the conjecture (1.21) using as Λ_ν the values given in Table 1.1 for each ν

here a_n, $a_n^\dagger$ and the fermionic creation and annihilation operators and h, $A > 1$, $0 \leq \nu \leq 1/2$ are constants.

This problem is at present under investigation, but some preliminary results seem to indicate that the previous techniques can be applied and the entanglement entropy of its ground state do indeed grow sublogarithmically.

Acknowledgements Research partially supported by grants 2016-E24/2, DGIID-DGA and FPA2015-65745-P, MINECO (Spain). FA is supported by FPI Grant No. C070/2014, DGIID-DGA/European Social Fund. The authors thankfully acknowledge the resources from the supercomputer *Memento*, technical expertise and assistance provided by BIFI (Universidad de Zaragoza).

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Chapter 2
Bulk-Edge Dualities in Topological Matter

Manuel Asorey

Abstract Novel bulk-edge dualities have recently emerged in topological materials from the observation of some phenomenological correspondences. The similarity of these dualities with string theory dualities is very appealing and has boosted a quite significant number of cross field studies. We analyze the bulk-edge dualities in the integer quantum Hall effect, where due to the simpler nature of planar systems the duality can be analysed by powerful analytic techniques. The results show that the correspondence is less robust than expected. In particular, it is highly dependent of the type of boundary conditions of the topological material. We give a formal proof of the equivalence of bulk and edge approaches to the quantization of Hall conductivity for metallic plates with local boundary conditions. However, the proof does not works for non-local boundary conditions, like the Atiyah-Patodi-Singer conditions, due to the appearance of gaps between the bulk and edge states.

2.1 Introduction

Topological matter is a new state of matter which includes topological quantum phases, topological insulators and topological semimetals. The field has undergone an impressive development in the last years, motivated by its potential applications to spintronics and quantum computation.

One interesting characteristic of some of the new topological materials is that its bulk is insulating while its edge is metallic. This striking property is made possible by the appearance of edge states. The quantized conducting properties of these materials are usually characterized by topological indices that either depend on the bulk observables of the material or on the number of edge states with special characteristics [1, 2] (see also [3]). The amazing coincidence of the two ways of computing the quanta of conductivity is sometimes attributed to a mysterious bulk-edge cor-

M. Asorey (✉)
Centro de Astropartículas y Física de Altas Energías, Departamento de Física Teórica, Universidad de Zaragoza, 50009 Zaragoza, Spain
e-mail: asorey@unizar.es

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_2

respondence. The appealing characteristics of such a correspondence has been in some cases related to the AdS/CFT duality that arises from string theory supporting a generalized holographic principle. The AdS/CFT correspondence is more explicit in 2+1 dimensions, where it becomes a real bulk-edge correspondence [4]. In this note we explore the bulk-edge correspondence in topological materials in some cases where there is an analytic control of the phenomenon. As in the case of string theory the phenomenon becomes simpler in lower dimensional systems like planar metallic plates. In two dimensions finite size effects appear to play an essential role in the analysis of the degeneracy of the ground state of magnetic systems by means of the Atiyah-Patodi-Singer (APS) index theorems [5]. However, the connection between the roles of edge and bulk states is not so evident in the derivation of the quantization of the electric conductivity. In this note we address such a problem in the case of integer quantum Hall effect. In particular, we analyze the stability of the integer character of the topological bulk index for finite planar metallic plates. showing that, in fact, the robustness of the quantization of the Hall conductivity does not rely only on bulk states. The contribution of edge states is essential for such a phenomenon, and the final result is highly dependent on the type of boundary conditions of the system.

2.2 Hall Effect in Planar Systems

Although the quantum physics of ordinary metals is described by non-relativistic quantum mechanics the same phenomenon appears in relativistic systems and in some non-relativistic systems like graphene where its low energy behavior is described by an effective relativistic system. Let us consider a massless Dirac fermion in a planar geometry. The Hamiltonian is given by

$$H_1 = i \not{D}_A \tag{2.1}$$

where

$$\not{D}_A = \sum_{j=1}^{2} \sigma^j (\partial_j - ieA_j) \tag{2.2}$$

and σ^j, $i = 1, 2$ are Pauli matrices and we have normalized the effective speed of light and the Planck constant ($c = \hbar = 1$). The electromagnetic potential A_j in the case of a constant transverse magnetic field B can be given by $A_1 = \frac{\varepsilon_1}{e}$, $A_2 = Bx^1 + \frac{\varepsilon_2}{e}$, where ε_j, $j = 1, 2$ are two arbitrary constants and e is the charge of the electron.

The spectrum of this Hamiltonian was found by Landau to be infinitely degenerated and quantized $E_n^{\pm} = \pm\sqrt{2eBn}$, $n \in \mathbb{N}$. This quantization of the Hamiltonian spectrum is on the roots of the integer quantum Hall effect. In fact, the square of the Dirac Hamiltonian is one half the standard non-relativistic Hamiltonian of the Hall effect

$$H_2 = -\tfrac{1}{2}\not{D}_A^2 = -\tfrac{1}{2}\sum_{j=1}^{2}(\partial_j - ieA_j)^2 + \tfrac{1}{2}eB\sigma_3, \tag{2.3}$$

with energy spectrum

$$E_n^{\pm} = eB(n+\tfrac{1}{2}) \pm \tfrac{1}{2}eB = \tfrac{1}{2}eBm_{\pm}, \tag{2.4}$$

where $m_+ = n+1$ and $m_- = n$. The existence of discretized energy levels implies the insulating character of the metal due to the effect of the magnetic field. However, for finite size metallic plates the situation can change due to the action of the edges.

What is remarkable is that even in absence of edges it is possible to infer the quantization of the Hall conductivity. The argument is due to Thouless et al. [1]. If we consider the Hall system in a torus $\mathbb{T}^2$ the consistency conditions require a quantization of the magnetic flux, i.e. for a torus with unit radius the magnetic field is quantized $eB = \frac{k}{2\pi}$ in terms of integers $k \in \mathbb{Z}$ [6]. In such a case the spectrum of the Hall Hamiltonian H_2 is discrete $E_n^{\pm} = |k|(n+\frac{1}{2}) \pm \frac{1}{2}|k|$ and independent of the magnetic phases ε_j, $j = 1, 2$. However, the eigenstates $\psi_n^{\pm l}$ do depend on those phases. The degeneracy of the different energy levels is $2|k|$, except for the vacuum state $n = 0$ with vanishing energy, where the degeneracy is simply $|k|$. The existence of zero-modes is guaranteed by the Atiyah-Singer index theorem. The eigenmodes of the spin σ_3 operator are called chiral states. The index theorem tell us that the difference between the numbers of zero modes with positive (ν_+) and negative (ν_-) chiralities is given by the Chern class defined by the magnetic field on the torus (see also [7])

$$\nu_+ - \nu_- = \frac{1}{2\pi}\int_{\mathbb{T}^2} F = k. \tag{2.5}$$

where $F = edA$ and

$$\nu_{\pm} = \dim\{\psi \in \ker \not{D}_A, \sigma_3\psi = \pm\psi\}. \tag{2.6}$$

Now, since for $k > 0$, $\nu_- = 0$ and for $k < 0$, $\nu_+ = 0$ we have that

$$\dim \ker \not{D}_A = \nu_+ + \nu_- = |k|, \tag{2.7}$$

i.e. the zero modes are chiral and its degeneracy is half of that of higher energy modes.

The observation of Thouless et al. is that the Hall conductivity can be given in terms of Landau states by Thouless et al. [1]

$$\sigma_{xy}^k = -\frac{ie^2}{4\pi^2}\sum_{n=0}^{\nu}\sum_{l=0}^{|k|-1}\int_{\widehat{\mathbb{T}}^2}\int_{\mathbb{T}^2}\left[(\partial_{\varepsilon_1}\psi_n^l)^*\partial_{\varepsilon_1}\psi_n^{l'} - (\partial_{\varepsilon_1}\psi_n^{l'})^*\partial_{\varepsilon_1}\psi_n^l\right], \tag{2.8}$$

where ν is the highest integer with $E_\nu < E_F$ and $\widehat{\mathbb{T}}^2$ is the dual torus of harmonic forms, which is parametrized by the fluxes $(\varepsilon_1, \varepsilon_2) \in (0, \frac{1}{k}) \times (0, \frac{1}{k})$ of the magnetic field. ν is also the number of Landau levels that are completely filled of electrons. Now, Hall conductivity σ^k_{xy} is up to a constant nothing but ν times the first Chern class of the Fourier-Mukai transform of the complex bundle $E^k(\mathbb{T}^2, \mathbb{C})$ defined by the magnetic field [8]. It is well known that for the first Landau energy level the Fourier-Mukai transform interchanges the rank and the Chern class of the bundles, mapping in this case a rank 1 bundle with first Chern class k into a rank k bundle with unit first Chern class [9–11]. The transformation can be also applied to higher Landau energy levels which finally leads to a vector bundle with Chern class ν when restricted to the filled Landau levels. In this sense, the quantization of Hall conductivity

$$\sigma^k_{xy} = \frac{e^2}{2\pi}\nu \tag{2.9}$$

is just a consequence of the Fourier-Mukai duality [12]. Although a metallic torus can be built, it is not possible to generate a constant magnetic field across it because it will require a ring of magnetic monopoles. However, an effective torus appears for infinite metallic plates, because in such a case the Landau spectral problem on the plane (2.4) can be mapped by Floquet-Bloch theorem into the spectral problem of a continuous family of spectral problems (2.3) on a unit torus with arbitrary magnetic fluxes $\varepsilon_1, \varepsilon_2 \in (0, 2\pi)$. Since the spectrum of the operators (2.4) does not depend on the fluxes $\varepsilon_1, \varepsilon_1 \in (0, 2\pi)$, the spectral bands reduce to discrete points like in Fig. 2.1. In this sense, the quantization of the conductivity in infinite metallic plates can be fully characterized in physical terms by bulk properties.

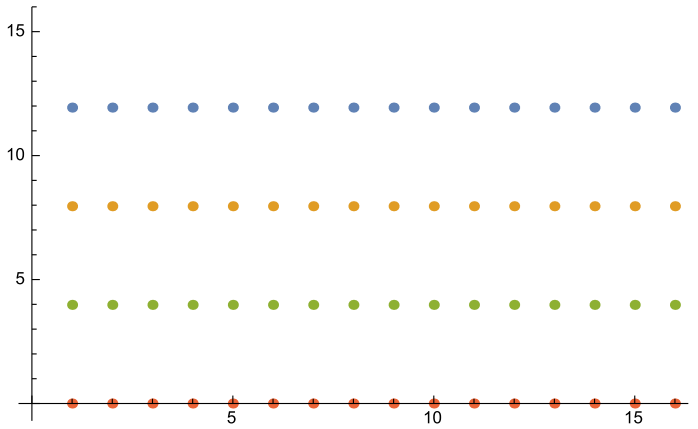

Fig. 2.1 Landau levels for a magnetic field $eB = 25/2\pi$ and arbitrary magnetic fluxes $(\varepsilon_1, \varepsilon_2)$

2.3 Boundary Effects and Atiyah-Patodi-Singer Theorem

One question which immediately arises is how this quantization can be maintained in cases where the magnetic flux across the plate is not quantized. The answer can be given in terms another index theorem, the Atiyah-Patodi-Singer theorem [5]. Let us consider an infinitely long metallic strip of unit width. Due to the translation invariance along the infinite direction of the strip one can identify by Floquet-Bloch theory the spectrum of the Dirac operator with that of the same operator on a cylinder of unit radius and arbitrary magnetic flux around the the compact direction, i.e.

$$-i\not{D}_A = -i\sigma_1(\partial_x) - i\sigma_2(\partial_\varphi + i\varepsilon_2 + i2\pi eBx) \tag{2.10}$$

with $x \in [0, 1]$ and $\varphi \in [0, 2\pi]$ (Fig. 2.2).

Now, the operator $-i\not{D}$ is symmetric in the space of spinors with compact support, but to become selfadjoint we must introduce appropriate boundary conditions at the edges of the cylinder. The most general boundary conditions are given by Asorey et al. [13, 14]

$$\begin{pmatrix} 1-\sigma_2 & 0 \\ 0 & 1+\sigma_2 \end{pmatrix} \begin{pmatrix} \psi_{S_1^1} \\ \psi_{S_0^1} \end{pmatrix} = U \begin{pmatrix} \sigma_3(1+\sigma_2) & 0 \\ 0 & \sigma_3(1-\sigma_2) \end{pmatrix} \begin{pmatrix} \psi_{S_1^1} \\ \psi_{S_0^1} \end{pmatrix}, \tag{2.11}$$

where U is any unitary operator acting on the boundary Hilbert space of spinors $L^2((S_1^1 \times S_0^1), \mathbb{C})$ commuting with σ_2, and $\psi_{S_1^1}$ and $\psi_{S_0^1}$ are the boundary values of the spinors at the two ends of the cylinder. The APS boundary conditions are given by

$$\prod_+^j \psi_{S_i^1} = 0, \qquad j = 0, 1, \tag{2.12}$$

where $\prod_+^j$ are the orthogonal projectors to the subspaces of non-negative eigenvalues of the boundary Dirac operators

$$\not{D}_{S_j^1} = -i\sigma_2(\partial_\varphi + i\varepsilon_2 + ij2\pi eB)$$

on the Hilbert spaces of boundary spinors $L^2(S_j^1)$ for $j = 0, 1$. The APS boundary conditions are highly non-local. Because of the anticommutation of σ_3 with the boundary operators $\not{D}_{S_i^1}$ we also have that

Fig. 2.2 Cylindric space

$$\Pi^j_- \sigma_3 \psi_{S^1_j} = 0, \qquad j = 0, 1, \tag{2.13}$$

where Π^j_- are the orthogonal projectors to the subspaces $\mathscr{H}^-_j$ of non-positive eigenvalues of $\not{D}_{S^1_j}$. In the splitting of the Hilbert space of boundary Dirac spinors $\mathscr{H}_j = L^2(S^1_j, \mathbb{C}^2) = \mathscr{H}^+_j \oplus \mathscr{H}^-_j$ into the orthogonal subspaces of the non-positive and positive eigenvalues of $\not{D}_{S^1_j}$, the unitary operator corresponding to the APS boundary conditions (2.13) is

$$U = \begin{pmatrix} \Pi^1_- & 0 & 0 & 0 \\ 0 & \Pi^1_- - 1 & 0 & 0 \\ 0 & 0 & \Pi^0_- & 0 \\ 0 & 0 & 0 & \Pi^0_- - 1 \end{pmatrix} \tag{2.14}$$

The APS boundary conditions break chiral symmetry of the Dirac operator because the boundary condition is not invariant under chiral symmetry.

$$\sigma_3 \Pi^j_+ = \Pi^j_- \sigma_3, \quad j = 0, 1.$$

The main reason for choosing APS boundary conditions is that with them the Dirac operator is not only a selfadjoint operator but also elliptic which allow it to satisfy the APS theorem [5].

The APS theorem generalizes the Atiyah-Singer theorem for manifolds with boundaries and establish that the difference of the numbers of zero modes of the Dirac operator with different chiralities can be expressed in analytic terms as

$$\nu_+ - \nu_- = \frac{1}{2\pi} \int_{[0,1]\times S^1} F + \frac{1}{2}[h(\not{D}_{S^1_1}) - h(\not{D}_{S^1_0}) + \eta(\not{D}_{S^1_1}) - \eta(\not{D}_{S^1_0})], \tag{2.15}$$

where $h(\not{D}_{S^1_i}) = \dim \ker \not{D}_{S^1_i}$, $i = 0, 1$, and $\eta(\not{D}_{S^1_i})$ is the eta invariant of $\not{D}_{S^1_i}$ given by its spectral asymmetry, which formally is defined by

$$\eta(\not{D}_{S^1}) = \sum_{\lambda \in \mathrm{Sp}\, \not{D}_{S^1}} \operatorname{sign} \lambda = \sum_{\lambda \in \mathrm{Sp}\, \not{D}_{S^1}} \frac{\lambda}{|\lambda|}. \tag{2.16}$$

The kernel of $\not{D}_{S^1_0}$ is trivial ($h(\not{D}_{S^1_0}) = 0$) whenever $\varepsilon_2 \notin \mathbb{Z}$ and one-dimensional ($h(\not{D}_{S^1_0}) = 1$) otherwise. In a similar manner $h(\not{D}_{S^1_0})$ also vanishes whenever $\varepsilon_2 + 2\pi e B \notin \mathbb{Z}$ and $h(\not{D}_{S^1_0}) = 1$ otherwise. The calculation of the η invariants is more involved, There are two ways of obtaining the value η. One is from the analytic continuation to $s = 0$ of the analytic regularization definition

$$\eta(\not{D}_{S^1_0}) = \sum_{m\in\mathbb{Z}} \frac{\text{sign}(m+\varepsilon)}{(m+\varepsilon)^s}\bigg|_{s=0} \qquad \varepsilon \notin \mathbb{Z},$$
$$\eta(\not{D}_{S^1_1}) = \sum_{m\in\mathbb{Z}} \frac{\text{sign}(m+\varepsilon+2\pi eB)}{(m+\varepsilon+2\pi eB)^s}\bigg|_{s=0} \qquad \varepsilon + 2\pi eB \notin \mathbb{Z}. \tag{2.17}$$

Another method is based on the identification of η with the imaginary part of the zeta function of the determinant of the Dirac operator

$$\eta(\not{D}_{S^1_i})] = -\frac{1}{2}\text{Im log det } \not{D}_{S^1_i}. \tag{2.18}$$

Both methods give the same results [15, 16]

$$\eta(\not{D}_{S^1_0})] = \varepsilon_2 - [\varepsilon_2], \qquad \eta(\not{D}_{S^1_1})] = \varepsilon_2 + 2\pi eB - [\varepsilon_2 + 2\pi eB], \tag{2.19}$$

when $\varepsilon_2 \notin \mathbb{Z}$ and $\varepsilon_2 + 2\pi eB \notin \mathbb{Z}$. The brackets $[\varepsilon]$ mean the integer part of ε

Now, since by Stokes theorem

$$\int_{[0,1]\times S^1} F = e\int_{S^1_1} A - e\int_{S^1_1} A = 2\pi eB, \tag{2.20}$$

we have

$$\nu_+ - \nu_- = [\varepsilon_2 + 2\pi eB] - [\varepsilon_2]. \tag{2.21}$$

Since $\nu_\pm = 0$ when $\mp B \geq 0$, the total number of zero modes of the Dirac operator is

$$\nu = \nu_+ + \nu_- = [\varepsilon_2 + 2\pi eB] - [\varepsilon_2] = |[\varepsilon_2 + 2\pi eB] - [\varepsilon_2]|. \tag{2.22}$$

Notice that the number of zero modes is always a positive integer even when the magnetic flux crossing the plate is not an integer multiple of the Bohr quantum. To some extent the contribution of the boundary supplements the external magnetic flux to reach the nearest integer quantum value. This result is also independent of the ambiguities that arise in the calculation of the spectral asymmetry η of the boundary Dirac operators [17].

The full spectrum of half the square of Dirac operator $H_2 = \frac{1}{2}\not{D}_A^2 = -\frac{1}{2}\Delta_A + eB\sigma_3$ is displayed in Fig. 2.3. The Landau levels get modified and the most significative effect is the appearance of edge states which are localized near the boundaries and whose energies interpolate between the different levels of the infinite dimensional cylinder.

Notice that since chiral symmetry is broken by the APS boundary conditions there is no paring between positive and negative eigenvalues of the spectrum of the Dirac operator $\not{D}_A$. In the lowest Landau level all eigenstates have the same chirality as the sign of the magnetic field B, whereas the nearest edge states have the opposite chirality. We also remark the bending of the high energy levels with respect

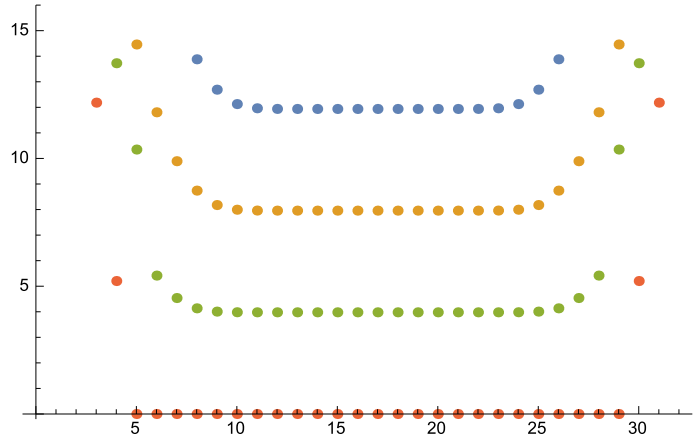

Fig. 2.3 Landau spectrum of the $H_2 = \frac{1}{2}\not{D}_A^2$ operator in a cylinder for a magnetic field $eB = 25/(2\pi)$ with APS boundary conditions and vanishing magnetic fluxes ($\varepsilon_2 = 0$)

to their values for an infinite plate. However, as already pointed out the APS theorem guarantees that there is no bending for the ground state.

From a physical viewpoint APS boundary conditions are not realistic for ordinary metals. Physical boundary conditions are *local* unlike the APS boundary conditions, i.e. U is a finite dimensional matrix acting only on spinor indices. Among local boundary conditions a simple type of chiral boundary conditions is given by

$$U = e^{2i \arctan e^{\theta}} \mathbb{I}. \tag{2.23}$$

The corresponding conditions

$$\begin{pmatrix} \sigma_1 + i e^{\theta\sigma_3}\sigma_3 & 0 \\ 0 & -\sigma_1 + i e^{\theta\sigma_3}\sigma_3 \end{pmatrix} \begin{pmatrix} \psi_{S_1^1} \\ \psi_{S_0^1} \end{pmatrix} = 0 \tag{2.24}$$

are known as chiral bag boundary conditions [13]. In the particular case $\theta = 0$, $U = iI$ one gets the Dirichlet boundary condition for the upper component of the Dirac spinor,

$$(I + \sigma_3)\psi_{S_1^1} = (I + \sigma_3)\psi_{S_0^1} = 0. \tag{2.25}$$

The Landau spectrum in this case is displayed in Fig. 2.4. A remarkable difference with the spectrum of APS boundary conditions is that the ground state is not degenerate pointing out that the APS theorem does not hold with local boundary conditions. Another difference is that in this case there is no clear splitting between edge and bulk states, which is manifest in the existence of a continuous interpolation between central and marginal states unlike in the APS case where there are large gaps between these states [18].

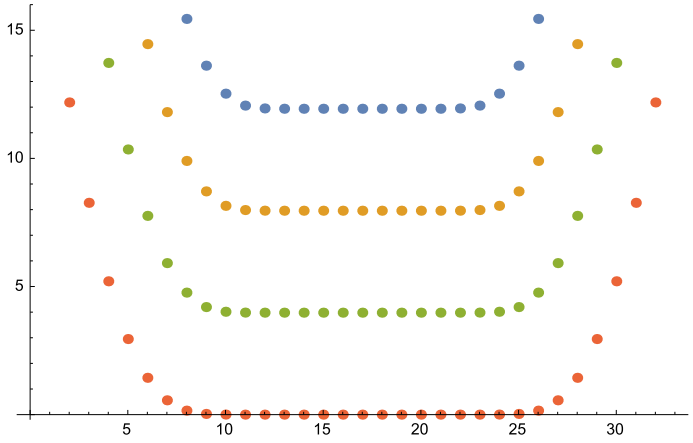

Fig. 2.4 Landau spectrum in a cylinder for a magnetic field $eB = 25/(2\pi)$ with local boundary conditions ($\theta = 0$) and null extra magnetic fluxes ($\varepsilon_2 = 0$) across the cylinder

2.4 Quantization of the Hall Conductivity

The action of a constant electric field E along the axis of the cylinder modifies the Hamiltonian[1]

$$H_3 = \tfrac{1}{2}\not{D}_A^2 + \tfrac{1}{2}eEx$$

introducing an slight tilt into its spectrum (see Fig. 2.5) which mixes the spectral bands and generates a current along the cylinder.

The Hall conductivity

$$\sigma_{xy} = \frac{I_\varphi}{2\pi E}$$

measures the ratio of the induced transverse current I_φ per unit area and the applied electric field E. The transverse current is given by the sum over all occupied states with energies below the Fermi level E_F, i.e over all eigenstates ψ_{nj} of H_3 with energies $E_{nj} < E_F$

$$I_\varphi = -i \sum_{n,j}^{E_{nj}<E_F} \int_{[0,1]\times S^1} \psi^*_{nj}(\partial_\varphi + i\varepsilon_2 + i2\pi eBx)\psi_{nj} = \sum_{n,j}^{E_{nj}<E_F} \int_{[0,1]\times S^1} \psi^*_{nj}\partial_{\varepsilon_2} H_3)\psi_{nj}$$

Now, since the eigenstates ψ_{nj} are normalized,

$$\int_{[0,1]\times S^1} (\partial_{\varepsilon_2}\psi^*_{nj}) H_3 \psi_{nj} + \int_{[0,1]\times S^1} \psi_{nj} H_3 \partial_{\varepsilon_2}\psi_{nj} = 0. \tag{2.26}$$

[1] From here on we assume a non-relativistic approximation to the interaction with the electric field which is closer to the phenomenological setup of the quantum Hall effect.

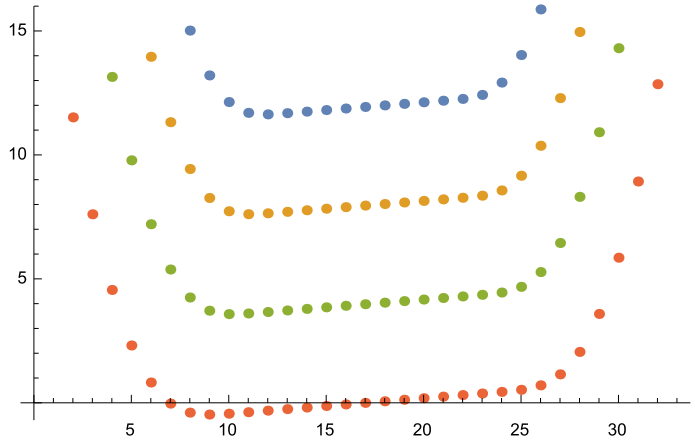

Fig. 2.5 Landau spectrum in a cylinder with magnetic field $eB = 25/(2\pi)$ and unit electric field ($eE = 1$) with local boundary conditions ($\theta = 0$) and null extra magnetic fluxes ($\varepsilon_2 = 0$) across the cylinder

Thus,

$$I_\varphi = \sum_{n,j}^{E_{nj}<E_F} \partial_{\varepsilon_2} \int_{\mathbb{C}^2} \psi^*_{nj} H_3 \psi_{nj} = \sum_{n,j}^{E_{nj}<E_F} \partial_{\varepsilon_2} E_{nj}. \tag{2.27}$$

This result holds for a compact cylinder $[0, 1] \times S^1$. However, as already mentioned usual physical systems do not have a cylindric form, they rather appear in the form of long strips. In such a case, assuming that the long direction of the strip is infinite, we can map the spectrum of the Hamiltonian by Floquet-Bloch theorem, into a continuous family of Hamiltonians $H_3^{\varepsilon_2}$ on the cylinder with magnetic fluxes $\varepsilon_2 \in (0, 1)$. In that case the spectrum becomes continuous because of the dependence on the magnetic fluxes ε_2 and is given by the union of a family of continuous Hall bands

$$\mathrm{Sp}\, H_3 = \bigcup_n^\infty \mathrm{Im}\, E_n,$$

where $E_n : S^1 \to \mathbb{R}$, $n = 0, \ldots, \infty$ are the real functions which describe the spectrum of Landau levels of H_3 on the cylinder for different values of the transverse magnetic flux $\varepsilon_2 \in S^1$. In this way the spectrum of the infinite plate fills the gaps between the dots in Fig. 2.5, and the intensity of the Hall current is

$$I_\varphi = \sum_{n=0}^\infty \int_{\varepsilon_n^-}^{\varepsilon_n^+} d\varepsilon_2 \partial_{\varepsilon_2} E_n, \tag{2.28}$$

where $\varepsilon_n^{\pm}$ are the two values of the magnetic flux where $E_n(\varepsilon_n^{\pm}) = E_F \pm eE$. Here is where the differences between the different types of boundary conditions appear. In the case of chiral boundary conditions (2.23) the curves $E_n(\varepsilon_2)$ are smooth due to the fact that the transition from edge to bulk states is continuous [19], and the Hall current is

$$I_\varphi = \sum_{n=0}^{\infty} \int_{\varepsilon_n^-}^{\varepsilon_n^+} d\varepsilon_2 \partial_{\varepsilon_2} E_n = \sum_{n=0}^{\infty} [E_n(\varepsilon_n^+) - E_n(\varepsilon_n^-)] = e^2 E \nu, \tag{2.29}$$

where ν is the number of filled Landau levels below the Fermi level. Thus, we obtain the same formula for quantized conductivity that in the bulk approach (2.9). However, in this case the contribution of both bulk and edge states is essential to keep the quantization constant for any value of the applied magnetic field B.

On the contrary in the case of APS boundary conditions there are discontinuities on those curves pointing out the existence of gaps dues to the sharp distinction between edge a bulk states. In particular, first Landau level degeneracy of bulk states is maximal thanks to the APS index theorem, whereas the first boundary states appear after a spectral gap. In this case the Formula (2.29) does not holds, due to the extra contributions of the discontinuities. In consequence, the quantization of the conductivity under APS boundary conditions does not follow the same pattern as that of chiral boundary conditions.

In some sense this result is the counterpart of the APS index theorem, which holds for APS boundary conditions, whereas it does not make any sense for chiral boundary conditions.

2.5 Conclusions

In summary, the correspondence bulk-edge that is very illuminating in holographic scenarios becomes very intricate in topological matter scenarios. We have analyzed the case of the integer quantum Hall where a detailed analysis can be performed. The results turn out to be highly dependent on the boundary conditions of the materials.

We have analyzed the quantization of Hall conductivity from standard bulk [1] and edge [2, 3] perspectives. The results do agree in the case of local boundary conditions because in such a case both approaches can be understood within a more general perspective that integrates both bulk and edge contributions. However, this compatibility only works for local boundary conditions because to some extent they do not neatly discriminate edge from bulk states. For boundary conditions where such a discrimination is more explicit, like the APS boundary conditions, bulk and edge quantizations lead to slightly different results.

It is also remarkable that the bulk-edge correspondence fails in scenarios where the APS index theorem preserves the degeneracy of the lowest Landau level whereas

it is manifest in scenarios where the APS theorem does not applies. This feature is not unrelated to the presence or not of clear identifications of edge states.

Generalizations to more general setups of topological matter like topological insulators of topological semimetals are not straightforward [20] and deserve further analysis.

Acknowledgements This work is partially supported by Spanish MINECO/FEDER grant FPA2015-65745-P and DGA-FSE grant E21-17R, and COST action program QSPACE-MP1405.

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Chapter 3
Near-Horizon Modes and Self-adjoint Extensions of the Schrödinger Operator

A. P. Balachandran, A. R. de Queiroz and Alberto Saa

Abstract We investigate the dynamics of scalar fields in the near-horizon exterior region of a Schwarzschild black hole. We show that low-energy modes are typically long-living and might be considered as being confined near the black hole horizon. Such dynamics are effectively governed by a Schrödinger operator with infinitely many self-adjoint extensions parameterized by $U(1)$, a situation closely resembling the case of an ordinary free particle moving on a semiaxis. Even though these different self-adjoint extensions lead to equivalent scattering and thermal processes, a comparison with a simplified model suggests a physical prescription to chose the pertinent self-adjoint extensions. However, since all extensions are in principle physically equivalent, they might be considered in equal footing for statistical analyses of near-horizon modes around black holes. Analogous results hold for any non-extremal, spherically symmetric, asymptotically flat black hole.

3.1 Introduction

The dynamics of quantum and classical fields in the vicinity of black holes have received considerable attention recently. Several aspects of the so-called soft photons theorems and the asymptotic symmetries in black hole spacetimes depend ultimately upon the dynamics and the underlying algebraic structure of test fields in the near-horizon region of black holes. For a recent comprehensive review on these subjects, see, for instance, [1]. Here, we revisit the case corresponding to the simplest clas-

A. P. Balachandran
Department of Physics, Syracuse University, Syracuse, NY 13244-1130, USA
e-mail: balachandran38@gmail.com

A. R. de Queiroz
Instituto de Física, Universidade de Brasília, C.P. 04455, Brasilia, DF 70919-970, Brazil
e-mail: amilcarq@unb.br

A. Saa (✉)
Department of Applied Mathematics, University of Campinas, Campinas, SP 13083-859, Brazil
e-mail: asaa@ime.unicamp.br

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_3

sical configuration of a field in the near-horizon region of a black hole: a massless Klein-Gordon field φ around a Schwarzschild black hole, which metric in standard coordinates reads

$$ds^2 = -\left(1 - \frac{2M}{r}\right) dt^2 + \frac{dr^2}{1 - \frac{2M}{r}} + r^2 d\Omega^2. \tag{3.1}$$

As we will see, massive scalar fields can be easily accommodated in our discussion, without altering our main conclusions. By exploring the standard decomposition for the scalar field

$$\varphi_{\ell m} = \frac{e^{-i\omega t}}{r} u_{\ell m}(r) Y_\ell^m(\theta, \phi) \tag{3.2}$$

and the usual tortoise coordinates

$$r_* = r + 2M \log\left(\frac{r}{2M} - 1\right), \tag{3.3}$$

one has the following effective Schrödinger equation for the radial function $u_{\ell m}$

$$\left(-\frac{d^2}{dr_*^2} + V_\ell(r)\right) u_{\ell m} = \omega^2 u_{\ell m}, \tag{3.4}$$

where the effective potential $V_\ell(r)$ is given by

$$V_\ell(r) = \left(1 - \frac{2M}{r}\right)\left(\frac{\ell(\ell+1)}{r^2} + \frac{2M}{r^3}\right), \tag{3.5}$$

which well known aspect is depicted in Fig. 3.1. The tortoise coordinate r_* runs over $(-\infty, \infty)$, with the near-horizon region corresponding to $r \to 2M$ and $r_* \to -\infty$, where the effective potential can be well approximated as

$$V_\ell(r_*) \approx V_\ell^{\text{nh}}(r_*) = \frac{\ell(\ell+1)+1}{4M^2 e} \exp\left(\frac{r_*}{2M}\right). \tag{3.6}$$

For $r \to \infty$, which corresponds to $r_* \to \infty$, the effective potential decreases as a power law. For scalar fields with mass $m_\varphi \neq 0$, there will be an extra term m_φ^2 inside the parenthesis of the second term in (3.5). It will not alter the effective potential exponential decay in the near-horizon region, nor the power law decay at infinity, although in this case $V_\ell \to m_\varphi^2$ for $r \to \infty$. Since the near-horizon potential (3.6) is not qualitatively altered by the mass term, our main conclusions will also hold for the massive case.

The effective Schrödinger equation (3.4) governs all dynamical processes involving scalar fields around Schwarzschild black holes. Scattering problems, in particular, involve certain boundary conditions at horizon and at infinity. In these problems, typically, one starts with a incoming wave from infinity which is scattered by the

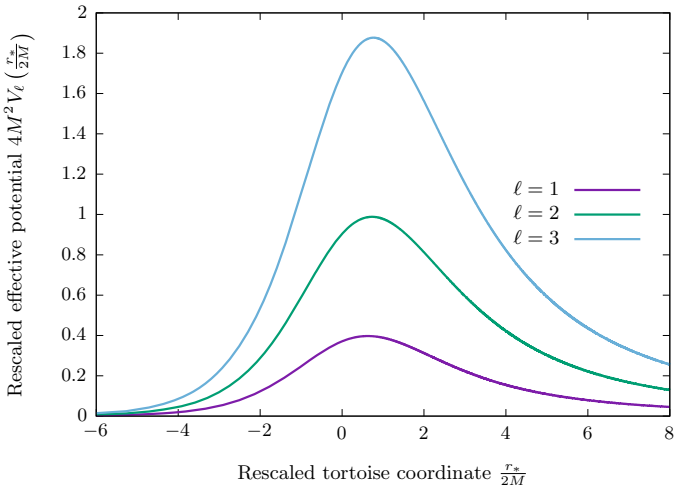

Fig. 3.1 Aspect of the effective potential $V_\ell(r_*)$ given by (3.5) for some values of ℓ. The potential decreases exponentially in the near-horizon region ($r_* \to -\infty$), see (3.6), and as a power law for $r_* \to \infty$ (the asymptotically flat region $r \to \infty$)

effective potential barrier (Fig. 3.1), leading to a reflected wave towards infinity and a transmitted wave that plunges into the black hole horizon. Such a typical situation corresponds to the following boundary conditions for $u_{\ell m}$

$$u_{\ell m}(r_*) = \begin{cases} A^{\text{in}}_{\ell m}(\omega)e^{-i\omega r_*} + A^{\text{out}}_{\ell m}(\omega)e^{i\omega r_*}, & r_* \to \infty, \\ B^{\text{in}}_{\ell m}(\omega)e^{-i\omega r_*}, & r_* \to -\infty. \end{cases} \tag{3.7}$$

The (complex) values of ω such that $A^{\text{in}}_{\ell m}(\omega) = 0$ are known to correspond to the so-called quasinormal modes, which dominate the asymptotic evolution of non-stationary configurations of the scalar field, see [2, 3] for comprehensive reviews on the subject. Here, we are interested in a different field configuration. We will consider processes which originate in the near-horizon region of the black hole and eventually are transmitted to the infinity through the potential barrier. This situation corresponds to the following boundary conditions

$$u_{\ell m}(r_*) = \begin{cases} A^{\text{out}}_{\ell m}(\omega)e^{i\omega r_*}, & r_* \to \infty, \\ B^{\text{in}}_{\ell m}(\omega)e^{-i\omega r_*} + B^{\text{out}}_{\ell m}(\omega)e^{i\omega r_*}, & r_* \to -\infty. \end{cases} \tag{3.8}$$

We will focus in the lower energy limit, which of course corresponds to small ω, which we assume to be positive. We will discuss the possibility of imaginary ω, which would correspond to negative eigenvalues ω^2 in the effective Schrödinger eigenproblem (3.4), in the last section. In the low-energy limit, we expect on physical grounds to have some oscillatory behavior in the near-horizon region and an exponential suppression, due to the effective potential barrier, as one departs from the horizon. It is rather natural to expect that $A^{\text{out}}_{\ell m} \to 0$ (or, to be more precise, $A^{\text{out}}_{\ell m}/B^{\text{out}}_{\ell m} \to 0$)

for small ω, and that the near-horizon modes $B^{\text{in}}_{\ell m}$ and $B^{\text{out}}_{\ell m}$ could be considered as long-living in the sense that the tunneling probability to infinity is extremely low, implying that near-horizon low-energy perturbations of the scalar fields tend to be confined near the black hole horizon. Moreover, since they are long-living and spatially confined, it is also natural to assume that such near-horizon modes could in principle attain thermal equilibrium, possibly with the black hole Hawking temperature $T_H = 1/8\pi M$.

Our analysis is based on the assumption that the dynamics of the near-horizon $B^{\text{in}}_{\ell m}$ and $B^{\text{out}}_{\ell m}$ modes, for small ω, can be well approximated by employing the Schrödinger operator

$$\mathcal{H} = -\frac{d^2}{dr_*^2} + V_\ell^{\text{nh}}(r_*) \tag{3.9}$$

on the domain $\left(-\infty, r_*^{\max}\right]$, for some finite $r_*^{\max}$ corresponding to a r not far from the horizon $r = 2M$. This is, of course, equivalent to assume that, for small ω, $A^{\text{out}}_{\ell m} = 0$, leading to a perfect reflection due to the effective potential barrier and, consequently, to a confinement of the near-horizon modes. This approach closely resembles the so-called "brick wall" proposal for the thermodynamical analysis of fields around black holes [4], even though we are concerned here with the dynamics in the interior region of the wall. As we will see, our approach may indeed be considered a generalization of the standard brick wall hypothesis.

It is a well known problem in standard Quantum Mechanics that the free-particle Schrödinger operator on the semiaxis has infinitely many self-adjoint extensions parameterized by a phase $\theta \in U(1)$, see [5, 6], for instance, for further references. We will show that similar results also hold for our problem, i.e., the Schrödinger operator (3.9) on the domain $\left(-\infty, r_*^{\max}\right]$ has infinitely many self-adjoint extensions determined by the boundary condition at $r_*^{\max}$. Moreover, all self-adjoint extensions in this case will give origin to physically acceptable descriptions for the near-horizon modes. Nevertheless, the comparison with a simplified model suggests a physical prescription to chose the pertinent extensions.

3.2 Self-adjoint Extensions of the Effective Schrödinger Operator

Let us introduce the dimensionless variable $x = r_*/2M$, in terms of which one has the following effective Schrödinger equation for near-horizon modes

$$\mathcal{H} u_{\ell m} = \left(-\frac{d^2}{dx^2} + \frac{c_\ell^2}{4} e^x\right) u_{\ell m} = \lambda^2 u_{\ell m}, \tag{3.10}$$

where

$$c_\ell^2 = \frac{4}{e}\left(\ell^2 + \ell + 1\right) \tag{3.11}$$

and $\lambda = 2M\omega$, which we assume initially to be positive. (The possibility of having imaginary λ will be discussed in the last section.) The functions $u_{\ell m}$ are defined over the domain $(-\infty, x^{\max}]$. As we will see, our conclusions are independent of the precise value of $x^{\max}$, provided, of course, it is finite. We will drop the indices ℓ and m for all functions and constants hereafter. It is natural to consider the initial domain $D(\mathcal{H})$ of the effective Schrödinger operator (3.10) as $C_0^\infty(-\infty, x^{\max}]$, i.e., the smooth (complex) functions u with compact support on the domain $(-\infty, x^{\max}]$. Notice that $\mathcal{H}$ is a symmetric operator with respect to the inner product

$$\langle v, u\rangle = \int_{-\infty}^{x^{\max}} \bar{v} u \, dx \tag{3.12}$$

since

$$\langle v, \mathcal{H}u\rangle = \langle \mathcal{H}v, u\rangle \tag{3.13}$$

for all $u, v \in D(\mathcal{H})$. However, it is clear too that $D(\mathcal{H}) \subset D(\mathcal{H}^\dagger)$ since (3.13) is valid also for functions $v \notin D(\mathcal{H})$, and this is the start point of the self-adjointness analysis of unbounded operators on Hilbert spaces [5, 6]. On physical grounds, we should expect $D(\mathcal{H}^\dagger)$ to be the set of all smooth functions with finite norm $||v|| = \sqrt{\langle v, v\rangle}$, or at least finite norm per length unit in order to accommodate some possible plane wave solutions. Hence, we will consider $D(\mathcal{H}^\dagger)$ as the set of smooth functions $v \in L^2(-\infty, x^{\max}]$, with the norm induced by (3.12). The von Neumann theorem assures that $\mathcal{H}$ will admit self-adjoint extensions provided the so-called deficiency index n_+ and n_- be equal and greater than zero, where $n_\pm$ are the dimension of the deficiency subspaces $N_\pm \subset D(\mathcal{H}^\dagger)$ defined by

$$N_\pm = \left\{ v \in D(\mathcal{H}^\dagger), \quad \mathcal{H}v = \pm i v \right\}. \tag{3.14}$$

In order to determine the deficiency subspaces $N_\pm$, notice that the change of variable $z = e^{\frac{x}{2}}$ reduces (3.10) to a modified Bessel equation, allowing us to write down the general solution of $\mathcal{H}v = \pm i v$ in terms of standard modified Bessel functions

$$v(x) = a I_{\mu_\pm}\left(ce^{\frac{x}{2}}\right) + b K_{\mu_\pm}\left(ce^{\frac{x}{2}}\right), \tag{3.15}$$

where a and b are constants and

$$\mu_\pm = \sqrt{2}\,(1 \mp i)\,. \tag{3.16}$$

From the standard asymptotic expressions for modified Bessel functions [7], one has for $x \to -\infty$

$$I_{\mu_\pm}\left(ce^{\frac{x}{2}}\right) \approx \frac{\left(\frac{c}{2}\right)^{\sqrt{2}(1\mp i)}}{\sqrt{2}\,(1\mp i)\,\Gamma\left(\sqrt{2}\,(1\mp i)\right)} e^{\frac{1\mp i}{\sqrt{2}}x} \tag{3.17}$$

and

$$K_{\mu_\pm}\left(ce^{\frac{x}{2}}\right) \approx \frac{1}{2}\left(\frac{c}{2}\right)^{\sqrt{2}(1\mp i)} \Gamma\left(\sqrt{2}\,(1\mp i)\right) e^{-\frac{1\mp i}{\sqrt{2}}x}. \tag{3.18}$$

It is clear that the modified Bessel function $K_{\mu_\pm}$ will give origin to solutions $v \notin D(\mathcal{H}^\dagger)$ since they will diverge exponentially for $x \to -\infty$. Hence, only the solutions involving $I_{\mu_\pm}$ are allowed, and we have $n_+ = n_- = 1$. The deficiency subspaces $N_\pm$ are then vector spaces with dimension 1 generated by $I_{\mu_\pm}$, and von Neumann theorem assures that $\mathcal{H}$ has a family of self-adjoint extensions parameterized by a phase $\theta \in U(1)$ [5, 6].

The structure of the differential operator $\mathcal{H}$ is rather simple and will allow us to determine explicitly all of its self-adjoint extensions $\mathcal{H}_\alpha$. Notice that, for smooth $u, v \in L^2\left(-\infty, x^{\max}\right]$, one has

$$\langle v, \mathcal{H}u\rangle - \langle \mathcal{H}v, u\rangle = \overline{v'}(x^{\max})u(x^{\max}) - \overline{v}(x^{\max})u'(x^{\max}), \tag{3.19}$$

from where we see that $\mathcal{H}$ will be self-adjoint provided

$$\frac{v(x^{\max})}{v'(x^{\max})} = \frac{u(x^{\max})}{u'(x^{\max})} = \alpha = \tan\frac{\theta}{2}, \tag{3.20}$$

with $\theta \in (-\pi, \pi)$, and we have finally established

$$D\left(\mathcal{H}_\alpha\right) = D\left(\mathcal{H}_\alpha^\dagger\right) = \left\{v \in L^2\left(-\infty, x^{\max}\right] \,\middle|\, v(x^{\max}) = \alpha v'(x^{\max})\right\}, \tag{3.21}$$

with $\mathcal{H}_\infty$ corresponding to the boundary condition $v'(x^{\max}) = 0$. It is worthy to notice that the case $\mathcal{H}_0$, which corresponds to $v(x^{\max}) = 0$, corresponds to the brick wall hypothesis [4]. Our analysis, besides of involving more general boundary conditions, is restricted to the other side of the wall, i.e. to the modes confined in the near-horizon region. Notice that the differential expression for the operator $\mathcal{H}_\alpha$ is independent of α, it alters only $D(\mathcal{H})$.

In order to interpret the physical meaning of the self-adjoint extensions $\mathcal{H}_\alpha$, let us consider now the eigenproblem (3.10) for positive λ. It has also solutions in terms of modified Bessel functions I_μ and K_μ, but now with pure imaginary order $\mu = 2i\lambda$. However, it is more convenient for our purposes here to write down the solution as a linear combination of $I_{2i\lambda}$ and $\overline{I_{2i\lambda}} = I_{-2i\lambda}$. One has

$$u(x) = a_\lambda I_{2i\lambda}\left(ce^{\frac{x}{2}}\right) + b_\lambda I_{-2i\lambda}\left(ce^{\frac{x}{2}}\right), \tag{3.22}$$

with a_λ and b_λ constants. For $x \to -\infty$, we have [7]

$$u(x) \approx \frac{a_\lambda\left(\frac{c}{2}\right)^{2i\lambda}}{2i\lambda\Gamma(2i\lambda)} e^{i\lambda x} - \frac{b_\lambda\left(\frac{c}{2}\right)^{-2i\lambda}}{2i\lambda\Gamma(-2i\lambda)} e^{-i\lambda x}, \tag{3.23}$$

from where one can read the scattering coefficients in the region very close to the horizon

$$B_\lambda^{\rm in} = -\frac{b_\lambda \left(\frac{c}{2}\right)^{-2i\lambda}}{2i\lambda\Gamma(-2i\lambda)}, \quad \text{and} \quad B_\lambda^{\rm out} = \frac{a_\lambda \left(\frac{c}{2}\right)^{2i\lambda}}{2i\lambda\Gamma(2i\lambda)}. \tag{3.24}$$

Defining the reflection coefficient as

$$R_\lambda = \frac{B_\lambda^{\rm in}}{B_\lambda^{\rm out}} = -\frac{b_\lambda}{a_\lambda}\frac{\Gamma(2i\lambda)}{\Gamma(-2i\lambda)}\left(\frac{c}{2}\right)^{-4i\lambda}, \tag{3.25}$$

we have

$$|R_\lambda| = \left|\frac{b_\lambda}{a_\lambda}\right|. \tag{3.26}$$

On the other hand, one can determine b_λ/a_λ from the boundary condition $u(x^{\rm max}) = \alpha u'(x^{\rm max})$. One has

$$\frac{b_\lambda}{a_\lambda} = -\frac{\chi}{\overline{\chi}} \tag{3.27}$$

where

$$\chi = I_{2i\lambda}\left(ce^{\frac{1}{2}x^{\rm max}}\right) - \frac{c\alpha}{2}e^{\frac{1}{2}x^{\rm max}} I'_{2i\lambda}\left(ce^{\frac{1}{2}x^{\rm max}}\right), \tag{3.28}$$

which clearly implies that $|R_\lambda| = 1$, meaning that, irrespective of the value of α, we have always full reflection of the near-horizon modes on the effective potential barrier, which is compatible with $A_\lambda^{\rm out} = 0$ as expected. From the scattering point of view, it is possible to implement a brick wall which effectively confine the modes in the near-horizon region without imposing $u(x^{\rm max}) = 0$. Moreover, any value of α is perfectly admissible in this context, all self-adjoint extensions give origin to physically acceptable descriptions for the near-horizon modes. We will have a complete set of (continuous) eigenvalues and eigenvectors for (3.10) for any value of α. As we will see below, all self-adjoint extensions will lead also to consistent thermodynamics for the near-horizon modes.

3.2.1 Statistical Mechanics and Thermal Equilibrium

All self-adjoint extensions $\mathcal{H}_\alpha$ describe confined incoming and outcoming near-horizon modes characterized by the coefficients $B_\lambda^{\rm in}$ and $B_\lambda^{\rm out}$, see (3.24). The probability of having incoming and outcoming modes with energy λ in the horizon are, respectively,

$$\left|B_\lambda^{\rm in}\right|^2 = \frac{\sinh 2\pi\lambda}{2\pi\lambda}|b_\lambda|^2, \quad \left|B_\lambda^{\rm out}\right|^2 = \frac{\sinh 2\pi\lambda}{2\pi\lambda}|a_\lambda|^2. \tag{3.29}$$

Notice that for small λ we have essentially $\left|B_\lambda^{\text{in}}\right|^2 \approx |b_\lambda|^2$ and $\left|B_\lambda^{\text{out}}\right|^2 \approx |a_\lambda|^2$. Let us suppose now that the near-horizon modes are at thermal equilibrium with temperature $T = \tau/2M$ (the Hawking temperature corresponds to $\tau = 1/4\pi$). Assuming a grand canonical ensemble and the detailed balance principle [8], we expect that incoming and outcoming modes be separately at thermal equilibrium, meaning that we should expect that both $|B_\lambda^{\text{in}}|^2$ and $|B_\lambda^{\text{out}}|^2$ obey Boltzmann distributions and, hence, both should be proportional to $e^{-\lambda/\tau}$. Interestingly, such detailed balance condition, which implies that incoming and outcoming modes are equally probable in a regime of thermal equilibrium, is compatible with any value of α, i.e., all self-adjoint extensions $\mathcal{H}_\alpha$ are equivalent also from the thermal equilibrium point of view. The compatibility is assured by the fact that $|a_\lambda|^2 = |b_\lambda|^2$ for any value of α, see (3.27) and (3.28). Hence, if one of the modes is assumed to be at thermal equilibrium, by (3.29) the other automatically be also at thermal equilibrium. It is fundamental for the detailed balance that the boundary condition implies

$$b_\lambda = e^{i\psi_\lambda} a_\lambda, \tag{3.30}$$

where the phase ψ_λ depends on all parameters of the problem, see (3.27) and (3.28), and particularly on the energy λ. Nevertheless, irrespective of the value of α, we have always $|a_\lambda|^2 = |b_\lambda|^2$.

3.2.2 A Prescription for the Extension Selection

Rigorously, for each value of α we have a fixed domain on the Hilbert space and a complete, physically consistent, description for the low-energy modes. We should not mix modes with different α since they belong to different domains. The physical interpretation of the parameter α is still rather unclear, but a simplified model can help to shed some light here. Let us consider the well-known elementary problem of the scattering by a rectangular barrier

$$V(x) = \begin{cases} 0, & x < 0, \\ V_0, & 0 \le x \le L, \\ 0, & x > L, \end{cases} \tag{3.31}$$

with both V_0 and L positives. We are interested on scattering problems of the type (3.8), i.e., on solutions of the type

$$u(x) = \begin{cases} B_\lambda^{\text{in}} e^{-i\lambda x} + B_\lambda^{\text{out}} e^{i\lambda x}, & x < 0, \\ C_\lambda e^{\sqrt{V_0 - \lambda^2}\, x} + D_\lambda e^{-\sqrt{V_0 - \lambda^2}\, x}, & 0 \le x \le L \\ A_\lambda^{\text{out}} e^{i\lambda x}, & x > L, \end{cases} \tag{3.32}$$

with $\lambda^2 < V_0$. The standard matching conditions at $x = 0$ and $x = L$ read

$$B^{\text{in}} + B^{\text{out}} = C_\lambda + D_\lambda, \tag{3.33}$$

$$-i\lambda\left(B^{\text{in}} - B^{\text{out}}\right) = \sqrt{V_0 - \lambda^2}(C_\lambda - D_\lambda), \tag{3.34}$$

$$A^{\text{out}}_\lambda e^{i\lambda L} = C_\lambda e^{\sqrt{V_0-\lambda^2}L} + D_\lambda e^{-\sqrt{V_0-\lambda^2}L}, \tag{3.35}$$

$$i\lambda A^{\text{out}}_\lambda e^{i\lambda L} = \sqrt{V_0 - \lambda^2}\left(C_\lambda e^{\sqrt{V_0-\lambda^2}L} - D_\lambda e^{-\sqrt{V_0-\lambda^2}L}\right). \tag{3.36}$$

After some straightforward algebra, one can evaluate the usual reflection coefficient R_λ leading to

$$|R_\lambda|^2 = \frac{V_0 \sinh^2\sqrt{V_0 - \lambda^2}L}{4\lambda^2(V_0 - \lambda^2) + V_0 \sinh^2\sqrt{V_0 - \lambda^2}L}. \tag{3.37}$$

The problem of near-horizon modes is mimicked in this toy model by assuming $L \to \infty$, which implies $|R_\lambda| \to 1$, i.e., full reflection leading to a "confinement" of the solutions (3.32) in the negative semiaxis. Since $|R_\lambda| \to 1$, we know that $A^{\text{out}}_\lambda \to 0$ and hence from (3.35) and (3.36) we have that $C_\lambda \to 0$, which implies the following condition for $u(x)$ on $x = 0$

$$u'(0) = -\sqrt{V_0 - \lambda^2}u(0). \tag{3.38}$$

Thus, finally, in the low-energy limit, $\lambda^2 \ll V_0$, we have that the dynamics of the totally reflect solutions for the barrier (3.31) may be viewed as an effective Schrödinger equation for a free particle on the negative semiaxis with the boundary condition corresponding to $\alpha^{-1} = -\sqrt{V_0}$. This simple results suggests that $\alpha^{-1} = -\sqrt{\max V_\ell}$ for the near-horizon modes. We would have different self-adjoint extensions for different angular momentum numbers ℓ, but this is hardly a surprise since the effective potential (3.5), and consequently the Schrödinger operator (3.10), does depend explicitly on ℓ. It is interesting to notice that the standard brick wall condition $\alpha = 0$ would require $\max V_\ell \to \infty$, which on the other hand demands $\ell \to \infty$. Nevertheless, all self-adjoint extensions act effectively as brick walls since we have full reflection for all values of α. In fact, despite our prescription for the selection of α, since all extensions are in principle physically equivalent, they might be considered in equal footing for statistical analyses of near-horizon modes around black holes.

3.3 Final Remarks

We will revisit in this last section two previously noticed points. First, that our results do not depend on the details of the Schwarzchild black hole. They will also hold for any non-extremal, spherically symmetric, static, and asymptotically flat black hole. The metric of a generic spherically symmetric static black hole can be cast in the form

$$ds^2 = -f(r)dt^2 + \frac{dr^2}{h(r)} + r^2 d\Omega^2. \tag{3.39}$$

The event horizon corresponds to the outermost zero of $f(r)$, say at $r = r_0$. The black hole is said to be non-extremal if $f'(r_0) = k > 0$, and hence in the vicinity of the horizon we have $f(r) \approx k_1(r - r_0)$. Regularity of the horizon area demands a smooth $\sqrt{-g}$, and from (3.39) we see also that $h(r) \approx k_2(r - r_0)$, with $k_2 > 0$. By using the standard decomposition (3.2) for the Klein-Gordon equation on the metric (3.39), we arrive to a Schödinger-like equation as (3.9), but now with the effective potential

$$\tilde{V}_\ell(r) = \ell(\ell+1)\frac{f}{r^2} + \frac{1}{2r}\left(f'h + fh'\right) \tag{3.40}$$

and tortoise coordinates such that

$$\frac{dr_*}{dr} = \frac{1}{\sqrt{fh}}. \tag{3.41}$$

If (3.39) is assumed to be asymptotically flat, we have $f(r) \to 1$ and $h(r) \to 1$ for $r \to \infty$, and hence (3.40) decays as a power law at infinity in the same way the Schwarzschild potential (3.5) does. On the other hand, in the near-horizon region one has

$$\tilde{V}_\ell(r) \approx k_1(r - r_0)\left(\frac{\ell(\ell+1)}{r_0^2} + \frac{k_2}{r_0}\right). \tag{3.42}$$

The new tortoise coordinate (3.41) also obeys $r_* \to -\infty$ on the horizon and, moreover, we have

$$r - r_0 = r_0 e^{\sqrt{k_1 k_2} r_*}, \tag{3.43}$$

from where we conclude that the effective potential (3.40) also decays exponentially in the near-horizon region. Indeed, the aspect of the generic effective potential (3.40) of a non-extremal, spherically symmetric, static, and asymptotically flat black hole is qualitatively the same of the Schwarzschild case, Fig. 3.1. All the analyses we have done follow analogously for the generic black hole case.

The second point corresponds to the imaginary λ case in (3.10). It is a well known and curious fact that the Schrödinger equation for the free particle on the semiaxis admits some bounded solutions, with negative energy, for certain self-adjoint extension choices, see [5]. We have the same interesting behavior here and they indeed correspond to the imaginary λ solutions of the eigenproblem (3.10). For $\lambda = \sigma i$, the fundamental solutions of (3.10) will be linear combinations of the modified Bessel functions $I_{2\sigma}$ and $K_{2\sigma}$. From the asymptotic behavior near the origin, we can discharge the second solution. Using the standard series expansion [7] for $I_{2\sigma}$, we have the following solution for the eigenproblem (3.10) with eigenvalue $\lambda^2 = -\sigma^2$,

$$u(x) = a_\sigma I_{2\sigma}\left(ce^{\frac{x}{2}}\right) = \sum_{k=0}^{\infty} \frac{e^{(k+\sigma)x}}{k!\Gamma(k+2\sigma+1)}\left(\frac{c}{2}\right)^{2(k+\sigma)}, \tag{3.44}$$

where it is assumed $\sigma > 0$. It is clear from (3.44) that $u(x)$ and all of its derivative are monotonically increasing functions and, thus, in order to accommodate such bounded solution for (3.10), a self-adjoint extension with $\alpha > 0$ is required, which will never be selected by our prescription. In our case, such bounded solutions do not oscillate, see (3.2), but rather decrease exponentially. This kind of overdamped evolution for scalar fields is quite similar to some highly damped quasinormal modes that are known to exist for generic black holes, see [9]. This topic is now under investigation.

Acknowledgements ARQ and AS thank the University of Zaragoza, where part of this work was carried on, for the warm hospitality. The authors acknowledge the financial support of CNPq and CAPES (ARQ and AS) and FAPESP (AS, Grant 2013/09357-9).

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Chapter 4
The Gauss Law: A Tale

A. P. Balachandran and A. F. Reyes-Lega

Abstract The Gauss law plays a basic role in gauge theories, enforcing gauge invariance and creating edge states and superselection sectors. This article surveys these aspects of the Gauss law in QED, QCD and nonlinear G/H models. It is argued that nonabelian superselection rules are spontaneously broken. That is the case with $SU(3)$ of colour which is spontaneously broken to $U(1) \times U(1)$. Nonlinear G/H models are reformulated as gauge theories and the existence of edge states and superselection sectors in these models is also established.

4.1 Introduction

This talk first discusses how locality enters the treatment of the Gauss law constraint and the gauge transformations of its generators, focussing on the Hamiltonian formalism. The important role of test functions in a proper treatment of Gauss law becomes apparent. Choices of various classes of test functions lead to various gauge groups of which the Gauss law-generated gauge group is an invariant subgroup. There are also gauge transformations of importance (at times loosely called "large gauge transformations") which are not connected to identity. Observables are local. A consequence is that they commute with all these gauge transformations. That leads naturally to a discussion of superselection rules and anomalies: the latter are just transformations which change the superselection sector and hence are spontaneously broken. These ideas are illustrated by examples such as axial anomalies and axial flavour transformations of the Standard Model.

We dedicate this article to our friend Alberto Ibort on the occasion of his sixtieth birthday.

A. P. Balachandran (✉)
Department of Physics, Syracuse University, Syracuse, NY 13244-1130, USA
e-mail: balachandran38@gmail.com

A. F. Reyes-Lega
Departamento de Física, Universidad de los Andes, A.A. 4976-12340 Bogotá, Colombia
e-mail: anreyes@uniandes.edu.co

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_4

We work with Minkowski spacetime $M^4 \cong \mathbb{R}^3 \times \mathbb{R}$, where $\mathbb{R}^3$ is the spatial slice. We also work in the gauge $A_0 = 0$. The gauge group is defined on the spatial slice $\mathbb{R}^3$.

4.2 The Structure of the Gauge Group: The Gauss Law

Let H be the group which is to be gauged. In QED, H is $U(1)$; in QCD, it is $SU(3)$.

The gauge group G is not H. Rather, its elements are maps g from $\mathbb{R}^3$ to H. If $g, h \in G$, the multiplication law is "point-wise": gh is defined by $(gh)(x) = g(x)h(x)$, $x \in \mathbb{R}^3$.

The Lie algebra $\mathscr{G}$ of the gauge group is associated with the Gauss law in quantum theory: the latter in Dirac's approach is a condition on state vectors $|\cdot\rangle$:

$$(D_i E^i + J_0)|\cdot\rangle = 0. \tag{4.1}$$

Here, E^i is the electric field, D_i the covariant derivative and J_0 is the charge density of the matter field. If λ_α is a basis of generators of the Lie algebra $\underline{H}$ of H, we can write

$$D_i E^i = \partial_i E^i + i A_i^\alpha E^{i,\beta}[\lambda_\alpha, \lambda_\beta], \quad E^i = E^{i,\alpha}\lambda_\alpha, \quad A_i = A_i^\alpha \lambda_\alpha, \quad J_0 = J_0^\alpha \lambda_\alpha, \tag{4.2}$$

where A_i^α, $E^{j,\beta}$ are canonically conjugate: at equal times,

$$[A_i^\alpha(x), E^{j,\beta}(y)] = i\delta_i^j \delta^3(x-y)\mathbb{I}. \tag{4.3}$$

These expressions are also valid for QED ($H = U(1)$).

The RHS of (4.3) is a distribution. Therefore, A_i^α, $E^{j,\beta}$ are operator-valued distributions. Derivatives of distributions are defined by smearing them with test functions and transferring derivatives to test functions. It turns out to be important to do so for the Gauss law (4.1).

Thus, let $S_0^\infty(\mathbb{R}^3)$ define $\underline{H}$-valued test functions $\Lambda = \Lambda^\alpha \lambda_\alpha$ on $\mathbb{R}^3$, Λ^α being real, infinitely differentiable and of fast decrease at infinity. (We will not be precise on the rate of decrease. It is to be adapted to the problem at hand.) We then write (4.1) as

$$\mathrm{Tr} \int \left[-(D_i \Lambda)E^i + \Lambda J_0\right]|\cdot\rangle = 0. \tag{4.4}$$

If $\mathrm{Tr}\,\lambda_\alpha\lambda_\beta = 2\delta_{\alpha\beta}$, we can also write (4.1) as

$$\int \left[-(D_i \Lambda)^\alpha E^{i,\alpha} + \Lambda^\alpha J_0^\alpha\right]|\cdot\rangle = 0. \tag{4.5}$$

In the Gauss law (4.4), it is important to choose Λ^α to vanish at infinity. It is only then that we can recover the classical Gauss law $D_i E^i + J_0 = 0$ by partial integration from (4.4) without generating surface terms.

4.3 The Group $\mathscr{G}_0^\infty$

The Gauss law generates infinitesimal gauge transformations dependent on x. We can see this as follows. Let

$$[\lambda_\alpha, \lambda_\beta] = 2i c^\gamma_{\alpha\beta} \lambda_\gamma. \tag{4.6}$$

Then,

$$D_i E^i = \partial_i E^{i,\alpha} \lambda_\alpha + 2i A^\alpha_i E^{i,\beta} c^\gamma_{\alpha\beta} \lambda_\gamma, \qquad D_i E^{i,\gamma} = \partial_i E^{i,\gamma} - 2A^\alpha_i E^{i,\beta} c^\gamma_{\alpha\beta}, \tag{4.7}$$

so that, for example,

$$[D_i E^{i,\gamma}(x), E^{j,\rho}(y)] = -2i E^{j,\beta}(x) c^\gamma_{\rho\beta} \delta^3(x - y). \tag{4.8}$$

This gives, for the smeared Gauss law,

$$\left[\int \left[-(D_i \Lambda)^\alpha E^{i,\alpha} + \Lambda^\alpha J^\alpha_0 \right], E^{j,\beta}(y) \right] = 2i \Lambda^\gamma(y) c^\gamma_{\rho\beta} E^{j,\rho}(y), \tag{4.9}$$

which is an infinitesimal y-dependent action of H.

Now, $\Lambda^\alpha(x) \to 0$ as $|x| \to \infty$, so that the Gauss law acts trivially at infinity. Hence, the group $\mathscr{G}_0^\infty$ it generates on exponentiation acts as identity at infinity (as indicated by the superscript ∞). The elements of $\mathscr{G}_0^\infty$ are also connected to identity as the subscript 0 indicates, since they are obtained by exponentiating a Lie algebra element.

If $U(h)$ is the operator representing $h \in \mathscr{G}_0^\infty$, we conclude that on physical states $|\cdot\rangle$,

$$U(h)|\cdot\rangle = |\cdot\rangle. \tag{4.10}$$

4.4 The Group $\mathscr{G}_0$: the Emergence of Global Groups

Let us denote the smeared Gauss law operator as $G(\Lambda)$:

$$G(\Lambda) = \int \mathrm{Tr} \left[-(D_i \Lambda) E^i + \Lambda J_0 \right], \qquad \Lambda \in S_0^\infty, \qquad G(\Lambda)|\cdot\rangle = 0. \tag{4.11}$$

We now consider more general operators $Q(\mu)$, where the test functions are not required to vanish at infinity:

$$Q(\mu) = \int \mathrm{Tr}\left[-(D_i\mu)E^i + \mu J_0\right], \qquad \mu \in \mathscr{C}^\infty. \tag{4.12}$$

If

$$\mu(x)\big|_{|x|\to\infty} = \mu \in \mathbb{R}, \tag{4.13}$$

there is no reason for $Q(\mu)$ to vanish on physical states. We call the group that the $Q(\mu)$'s generate as $\mathscr{G}_0$.

Now, $\mathscr{G}_0^\infty$ is a normal subgroup og $\mathscr{G}_0$. That follows from

$$[\mu, \Lambda] = 2i\mu^\alpha \Lambda^\beta c^\gamma_{\alpha\beta}\lambda_\gamma \in S_0^\infty \tag{4.14}$$

for $\mu = \mu^\alpha\lambda_\alpha$, $\Lambda = \Lambda^\beta\lambda_\beta$, since the RHS tends to zero as $|x| \to \infty$.

Consider the quotient group

$$\hat{H} = \mathscr{G}_0/\mathscr{G}_0^\infty. \tag{4.15}$$

It is a group that acts non-trivially on quantum states.

Let us assume that $(\mu - \mu_\infty) \in S_0^\infty$, that is, that μ approaches its asymptotic value rapidly. Then, if $g(\mu) \in \mathscr{G}_0$, $U(g(\mu))|\cdot\rangle$ depends only on μ_∞. That is because if $\mu_{1,\infty} = \mu_{2,\infty}$, $(\mu_1 - \mu_2) \in S_0^\infty$ and $G(\mu_1 - \mu_2)|\cdot\rangle = 0$.

The group $\hat{H}$ is in fact isomorphic to H in simple cases like QED or QCD. In these cases, we can choose $\mu(x) = \mu_\infty$ for all x and then

$$Q(\mu) = \int \mathrm{Tr}\,\mu_\infty\left(-A_i^\alpha E^{i,\beta}[\lambda_\alpha, \lambda_\beta] + J_0\right) \tag{4.16}$$

is the familiar H-generator after a normalisation of μ_∞, which for QED is $\mu_\infty = 1$. For QCD, we choose eight μ_∞'s, $\mu^\alpha_{\infty,\beta}\lambda_\alpha$ ($\beta = 1, 2, \ldots, 8$), where $\mu^\alpha_{\infty,\beta} = \delta^\alpha_\beta$. Equation (4.16) shows that non-abelian gluons carry non-abelian charges, as the first term in (4.16) is not zero. In QED, instead, the first term is zero, photons having no charge.

But $\hat{H}$ can differ from H. A good example is the't Hooft-Polyakov model, where $H = U(1)$ while, as Witten has shown [1], $\hat{H} = \mathbb{R}$ in the presence of magnetic monopoles. That leads to fractional charges for dyons.

4.5 The Sky Group $\hat{\mathscr{G}}_0$

We can now go one step further and consider the boundary condition

$$\mu(\boldsymbol{x}) = \mu(|\boldsymbol{x}|\hat{x}) \xrightarrow[|\boldsymbol{x}|\to\infty]{} \hat{\mu}(\hat{x}). \tag{4.17}$$

That is, allow μ to approach an angle-dependent limit at infinity. (We are "blowing up" infinity.) Then, we get the "Sky" group $\hat{\mathcal{G}}_0$ [2, 3] with generators

$$\hat{Q}(\hat{\mu}) = \int_{S^2_\infty} \mathrm{Tr}\left[-(D_i\hat{\mu})E^i + \hat{\mu}J_0\right]. \tag{4.18}$$

This group is of importance for discussing infrared effects [2].

4.6 Winding Number Gauge Transformations

These are gauge transformations h which approach $\mathbb{I}$ at infinity. Hence, they can be regarded as maps from S^3 to H. If h has winding number other than zero, then h is a winding number gauge transformation. We refer to [3] for the definition and properties of such maps h.

If H is $U(1)$ as in QED, then there is no h with non-zero winding number: $\Pi_3(U(1)_g) = 0$.

If H is a compact, simple Lie group like $SU(N)$, there are such transformations. Let h_1 be one such typical transformation with winding number one. Then, powers of h_1, namely h_1^k, $k \in \mathbb{Z}$, generate the group $\mathbb{Z}$.

If $\mathcal{G}_W^\infty$ is the gauge group with elements becoming identity at infinity, but not necessarily connected to identity, then the winding number group is $\mathcal{G}_W^\infty/\mathcal{G}_0^\infty$.

We can relax the condition at infinity and consider $\hat{\mathcal{G}}_W$. With $\hat{\mathcal{G}}_W$, we allow angle-dependence at infinity. This group may not be connected to identity. Then again we have that $\hat{\mathcal{G}}_W/\hat{\mathcal{G}}_0$ (the subscript 0 as usual denoting the component connected to identity) is the winding number group:

$$\hat{\mathcal{G}}_W/\hat{\mathcal{G}}_0 \approx \mathcal{G}_W/\mathcal{G}_0. \tag{4.19}$$

The winding number group ("deck transformations") is responsible for the θ-vacua of QCD.

An important point is that in QCD and $SU(N)$ gauge theories, we cannot write winding number operators in terms of field variables like A and E. (An exception occurs in the't Hooft-Polyakov model mentioned above.) Still, they are well-defined as automorphisms of local observables. There may be cases where they are not implementable as unitary operators, leading to their "spontaneous" breakdown.

We now have a list of various gauge groups with their mutual relations:

$$\begin{array}{ccccccc} \hat{\mathcal{G}}_W & \supset & \mathcal{G}_W & \supset & \mathcal{G}_0 & \supset \mathcal{G}_0^\infty = \text{Gauss law group} \\ \cup & & \cup & & \cup & & \\ \hat{\mathcal{G}}_W^\infty & = & \mathcal{G}_W^\infty & \supset & \mathcal{G}_0^\infty & & \end{array} \tag{4.20}$$

In each non-trivial inclusion here, the subgroup is normal. Only the Gauss law group necessarily acts as identity on quantum states. Also, groups with index W do not have operators given by the canonical approach in QCD.

4.7 On Local Observables and Gauge Invariance

Let $\mathscr{A}$ be the algebra of local observables. If φ is a local quantum field of the Lagrangian approach and f is a test function with compact support K, then

$$\varphi(f) = \int d^3x\, f(x)\varphi(x) \tag{4.21}$$

or, better, $e^{i\varphi(f)}$ is an element of $\mathscr{A}$. Here, for illustration, we assume that φ is a scalar. We can exponentiate $\varphi(f)$ in (4.21) to get a unitary (and hence bounded) operator.

In our approach, K is a spatial region. A more rigorous formulation will require K to be a spacetime region [4].

If $a \in \mathscr{A}$, thought of as an operator in a Hilbert space $\mathscr{H}$ of physical states, then we have that

$$aU(h) = U(h)a \qquad \text{if } h \in \mathscr{G}_0^\infty. \tag{4.22}$$

That is because we want both $|\cdot\rangle$ and $a|\cdot\rangle$ to be in the kernel of the Gauss law. Thus,

$$[a, G(\Lambda)] = 0 \qquad \text{if } \Lambda \in S_0^\infty. \tag{4.23}$$

The result (4.22) follows from here on exponentiation of $G(\Lambda)$.

But a is local. An important consequence is then that a commutes with all the $\mathscr{G}$-groups.

Let $\mathscr{A}'$ be the commutant of $\mathscr{A}$ and $\mathbb{C}\mathscr{G}_W$ the group algebra of $\mathscr{G}_W$. Then, the above claim means the following: because of locality and the Gauss law constraint, we have that

$$\mathscr{A}' \supseteq \mathbb{C}\mathscr{G}_W. \tag{4.24}$$

It is enough to show the infinitesimal version of this result for all $\mathscr{G}$'s except $\hat{\mathscr{G}}_W$'s (Towards the end of this section, we consider $\mathbb{C}\mathscr{G}_W$). For the former, there is the generator $Q(\mu)$. Let $\varphi(f)$ be a local field supported in a compact region K. The commutator $[Q(\mu), \varphi(f)]$ depends only on $\mu\big|_K$, the restriction of μ to K, because of locality. That is, if $\mu\big|_K$ and $\nu\big|_K$ are equal, then

$$[Q(\mu) - Q(\nu), \varphi(f)] = 0. \tag{4.25}$$

So let us extend $\mu\big|_K$ to a $\nu \in C_0^\infty$ in any manner with the only condition $\nu\big|_K = \mu\big|_K$. Then,

$$[Q(\mu), \varphi(f)] = [Q(\nu), \varphi(f)] = [G(\nu), \varphi(f)] = 0. \tag{4.26}$$

The second equality holds true because $\mu, \nu \in C_0^\infty$. This proves the result.

The proof for winding number transformation is along the same lines. If $g \in \hat{\mathscr{G}}_W$, then $U(g)\varphi(f)U^{-1}(g)$ depends only on $g\big|_K$ and $g^{-1}\big|_K$. We now extend $g^{-1}\big|_K$ outside K, so that it has globally zero winding number and belongs to $\mathscr{G}_0^\infty$. If the extended gauge transformation is h, then $U(h) \in \mathscr{A}'$. Hence, $U(g) \in \mathscr{A}'$ too. We can thus conclude that $\hat{\mathscr{G}}_W \in \mathscr{A}'$.

4.8 On Superselection Groups

These are the transformations commuting with $\mathscr{A}$. Hence, the group $\hat{\mathscr{G}}_W$ is associated with the superselection group.

The subgroup $\mathscr{G}_0^\infty$ of Gauss law becomes $\mathbb{I}$ on quantum states. It is normal in $\hat{\mathscr{G}}_W$. Hence, it is more appropriate to identify $\hat{\mathscr{G}}_W/\mathscr{G}_0^\infty$ or a subgroup thereof with the superselection group.

The group algebra $\mathbb{C}(\hat{\mathscr{G}}_W/\mathscr{G}_0^\infty)$ commutes with $\mathscr{A}$: $\mathbb{C}(\hat{\mathscr{G}}_W/\mathscr{G}_0^\infty) \in \mathscr{A}$, it is a Hopf algebra. For more discussions on Hopf algebras, see [5]. We can also work with $\mathbb{C}(\hat{\mathscr{G}}_W/\mathscr{G}_0^\infty)$ to illustrate superselection theory.

Subgroups of $\hat{\mathscr{G}}_W/\mathscr{G}_0^\infty$ give us the familiar superselection rules of QED and QCD. That is because of the following. Local observables cannot change the irreducible representation (IRR) ρ of $\hat{\mathscr{G}}_W/\mathscr{G}_0^\infty$ on the Hilbert space $\mathscr{H}_\rho$ (we now label $\mathscr{H}$ also with ρ): $\mathscr{A}\mathscr{H}_\rho \subseteq \mathscr{H}_\rho$. Hence, by definition, $\hat{\mathscr{G}}_W/\mathscr{G}_0^\infty$ is superselected.

More will be said below when the group in question is non-abelian. We now illustrate these remarks.

4.8.1 Charge and Colour

In QED, $\mathscr{G}_0/\mathscr{G}_0^\infty = U(1)$. Thus, charge is superselected. So is colour, since $\mathscr{G}_0/\mathscr{G}_0^\infty = SU(3)_c$ in QCD.

There is a subtlety about colour because it is non-abelian. In a unitary IRR (UIRR), as Dirac has explained, we can diagonalise a maximal commuting set (CCS) of operators from its group algebra $\mathbb{C}SU(3)$. A choice for the CCS is C_2, C_3, I, I_3, Y, where C_2, C_3 are the quadratic and cubic Casimir operators, I is isospin and I_3, Y are the operators representing $\lambda_3/2$ and $\lambda_8/\sqrt{3}$ of the Gell-Mann matrices. Thus, a vector state in a UIRR ρ is characterised by the eigenvalues c_2, c_3, i, i_3, y of these operators:

$$\mathscr{H}_\rho : \quad |c_2, c_3, i, i_3, y, \cdot\rangle. \tag{4.27}$$

No operator of $\mathscr{A}$ will change these eigenvalues. But a generic element of $SU(3)_c$ (for example, U_α and V_α, the $U-$ and $V-$ spin operators of [6]) will change i_3, y. Hence, they cannot be implemented on $\mathscr{H}_\rho$.
Operators changing $\mathscr{H}_\rho$ are said to be *spontaneously broken* or *anomalous*. Hence, in QCD, $SU(3)_c$ of colour is spontaneously broken to $S\left(U(1)_{I_3} \times U(1)_Y\right)$, generated by I_3, Y [2]. Analogous results have been found for the ethylene molecule [7] and for colour breaking by the non-abelian monopoles of grand unified theories [8–11].

Remark: We make no distinction between spontaneous symmetry breaking and symmetry breaking by anomalies. Both are of the same origin: they change the domain of the observables $\mathscr{A}$. In the above, anomalous operators change $\mathscr{H}_\rho$. (It was Esteve who first discussed anomalies as transformations changing the domain of the Hamiltonian [12].)

4.8.2 QCD θ-vacua

These originate in $\mathscr{G}_W$. It is enough to consider $\mathscr{G}_W^\infty$. Let T be a winding number one transformation. Then,

$$U(T)a = aU(T) \qquad \text{if } a \in \mathscr{A} \tag{4.28}$$

because of locality. It also preserves the Gauss law constraint: if $G(\Lambda)|\cdot\rangle = 0$, then $G(\Lambda)U(T)|\cdot\rangle = 0$. Hence, in an IRR of $\mathscr{A}$, we can diagonalise $U(T)$.

For $H = SU(2)$, a typical winding number one transformation is

$$T(\boldsymbol{x}) = \cos\theta(r) + i\boldsymbol{\tau}\cdot\hat{x}\sin\theta(r), \quad r = |\boldsymbol{x}|, \quad \theta(0) = -\pi, \quad \theta(\infty) = 0. \tag{4.29}$$

If T has winding number one, T^k has winding number k. So the group it generates is $\mathbb{Z}$. The UIRR's of $\mathbb{Z}$ are labelled by the points on a circle $S^1 = \{e^{i\theta}\}$. If the quantum state is characterised by $\rho_\theta : T \to U(T) = e^{i\theta}$, we have that

$$U(T)|e^{i\theta}, \ldots\rangle = e^{i\theta}|e^{i\theta}, \ldots\rangle. \tag{4.30}$$

These are the θ-states of QCD. There is an extensive literature on θ-states.

4.8.3 The Sky Group

This group emerged from the study of infrared problems in QED. The name was suggested by the Scri or BMS group of Bondi, Metzner and Sachs [13, 14] and the Spi group of Ashtekar [15].

The Sky group $\mathscr{G}$ has generators $Q(\mu)$, where

$$\mu(\boldsymbol{x}) = \mu(r\hat{n}) \xrightarrow[r\to\infty]{} \mu(\hat{n}), \tag{4.31}$$

and where $\mu(\hat{n})$ need not be zero.

There is an operator, an intertwiner, $V(\omega)$ which maps state vectors with $Q(\mu) = 0$ to ones where it is not zero. Thus, there are the sectors with "in" state vectors (cf. [16, 17] and references therein)

$$e^{q_n \int d^3x [A_i^-(x)\omega_i^+(x) - A_i^+(x)\omega_i^-(x)]} |n, P, \cdot\rangle := |n, P, \omega, \cdot\rangle, \tag{4.32}$$

$$|n, P, 0, \cdot\rangle \equiv |n, P, \cdot\rangle, \qquad q_n \neq 0 \tag{4.33}$$

created by the infrared photons. The first operator in (4.32) gives the intertwiner. Here $A_i^\pm$ are the positive and negative frequency parts of the electromagnetic potential in the Coulomb gauge, and the functions ω_i^+, $\omega_i^- = \bar{\omega}_i^+$ are transverse:

$$\partial_i \omega_i^\pm(x) = 0, \tag{4.34}$$

Also they do not vanish fast as we approach infinity:

$$\lim_{r\to\infty} r^2\, \hat{x}_i\, \omega_i(x)^\pm \neq 0. \tag{4.35}$$

One such typical ω_i^+ has the Fourier transform

$$\hat{\omega}_i^+(k) = \int d^3x\, e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \omega_i^+(x) = \frac{1}{P\cdot k + i\varepsilon}(P_i - \boldsymbol{P}\cdot\hat{k}\,\hat{k}_i) \tag{4.36}$$

(with ε decreasing to zero as usual). The momentum P_μ is the total momentum of the charged system. (We have not shown the individual momenta and charges of which P and q_n are composed as they are not important for our considerations.) The important point here is that $\hat{\omega}_i^+$ is not square-integrable:

$$\langle \omega, \omega\rangle := \lim_{|\boldsymbol{k}'|\to 0} \int_{|\boldsymbol{k}'|}^\infty \frac{d^3k}{2|\boldsymbol{k}|} |\hat{\omega}_i^+(k)|^2 = \infty. \tag{4.37}$$

It is then a theorem [18] that the representation of $\mathscr{A}$ built on (4.32) is superselected: it is not the Fock space representation.

$V(\omega)$ commutes with the Gauss law operator $G(\Lambda)$. But that is not the case with $Q(\mu)$:

$$e^{iQ(\mu)} V(\omega) = \exp\left[q_n \lim_{r^2\to\infty} \int_{S^2_\infty} d\Omega\, r^2 \mu(\hat{n}) \hat{n}_i (\omega_i^+ - \omega_i^-)(r\hat{n}) \right] V(\omega) e^{iQ(\mu)}, \tag{4.38}$$

where S^2_∞ is the "sphere" at infinity (we are "blowing up" infinity).

The algebra defined by the relation (4.38) is useful to study the infrared effects in gauge theories and their phenomenology [19].

There are non-abelian and gravitational generalisations of $V(\omega)$ [19]

If $|\cdot\rangle$ is a vector in the Fock space, then $V(\omega)|\cdot\rangle$ is not in the Fock space since ω_i is not square-integrable:

$$\int d^3x\, |\omega_i(x)|^2 = \infty. \tag{4.39}$$

Using this fact, one proves that Lorentz invariance is broken: boost operators cannot be defined on $V(\omega)|\cdot\rangle$. Colour and $SL(2,\mathbb{C})$ gauge symmetry are similarly broken. The discussion of these issues may be found in papers.

4.9 Global Symmetries: Lorentz and Flavour Groups

Apart from gauge groups, whose elements are spacetime dependent, we have in addition global symmetries. They transform *all* local fields and cannot be localised in a compact region K. A simple example is spatial translation. For a free scalar field, its generators are

$$P_i = \frac{1}{2}\int d^3\boldsymbol{x}\ [\varphi(x)\partial_i \Pi(x)]\,, \qquad [\varphi(x), \Pi(y)]\Big|_{x^0=y^0} = i\delta^3(\boldsymbol{x}-\boldsymbol{y}), \tag{4.40}$$

as deduced from the standard Lagrangian. They involve a density such as $\varphi(x)\partial_i\Pi(x)$ integrated over *all* space. For these reasons, they are not local. We call them *global*.

On local observables $\mathscr{A}$, global symmetries act as automorphisms. Unitary elements of $\mathscr{A}$ also act as automorphisms of $\mathscr{A}$. The latter generate the *inner* automorphism group Inn $\mathscr{A}$. If Aut $\mathscr{A}$ is the group of all automorphisms of $\mathscr{A}$, then Inn $\mathscr{A}$ is a normal subgroup of Aut $\mathscr{A}$. Global symmetries are elements of the quotient group Aut $\mathscr{A}$/Inn $\mathscr{A}$, which is called the outer automorphism group Out $\mathscr{A}$.

There is no guarantee that global symmetries, that is Out $\mathscr{A}$, can be implemented by operators in an IRR ρ of $\mathscr{A}$ on $\mathscr{H}_\rho$. Superselection operators are multiples of identity on $\mathscr{H}_\rho$ and it can happen that elements of Out $\mathscr{A}$ change ρ. In that case, they are spontaneously broken. We know many such examples. We list a few below.

4.9.1 Axial U(1) Anomaly

In quantum physics, we seek a representation of $\mathscr{A}$ which preserves the domain $\mathscr{D}_H$ of the Hamiltonian: $\mathscr{A}\mathscr{D}_H \subseteq \mathscr{D}_H$. This is important so that we have well-defined time evolution.

But, as Esteve discusses [12], axial $U(1)$ transformations $U(1)_A$ change $\mathscr{D}_H$, that is, the IRR of $\mathscr{A}$. Hence, they are spontaneously broken. That is so in QED and the Standard Model.

4.9.2 The Axial Flavour Anomaly

The flavour group in QCD at the Lagrangian level is $U(N_f)_L \times U(N_f)_R$ (upto discrete groups) acting on the left- and right-handed quarks. If (g, h) is a transformation of this group, they are interchanged by parity P:

$$P : \ (g, h) \to (h, g). \tag{4.41}$$

Vector transformations (g, g) commute with P. The axial transformations (g, g^{-1}) do not. The latter are all anomalous.

4.9.3 How QED Breaks Lorentz Invariance

A very striking example occurs in QED, where, as proved by Buchholz[1] [20] and Fröhlich, Morchio and Strocchi [21, 22], infrared effects dress the charged particle states by a $V(\omega)$ as in [21, 22], ω being known, and change the Fock space to a non-Fock space. In this new representation space, boost generators and hence the Lorentz group are spontaneously broken.[2] For an important generalization of these works, see [23].

There are extensions of this result to QCD [16].

4.9.4 The Higgs Field

The Higgs field is of standard use for the spontaneous breaking of symmetry. We discuss it briefly in the context of the group $U(1)$, such as in superconductivity.

So let ϕ be a charged Higgs field approaching the constant value ϕ_∞ at spatial infinity. If a is a local observable, then

[1] In [20], Buchholz has proven that Lorentz transformations must be spontaneously broken in electrically charged sectors and also that electrically charged states cannot be eigenstates of the mass operators.

[2] Fröhlich, Morchio and Strocchi base their work on the asymptotic fields (relying on Buchholz's collision theory for massless Bosons [24]). In [25], Buchholz relates the problem to the interacting (time zero) fields, i.e. Gauss law.

$$\lim_{r\to\infty}[a,\phi(x)]=0,\qquad r=|\boldsymbol{x}|, \tag{4.42}$$

so that ϕ_∞ is superselected.

We consider $U(1)$ as a gauge symmetry. So, if $u\in U(1)$, then

$$U(u)a=aU(u) \tag{4.43}$$

and $U(u)$ too commutes with all local observables.

But

$$U^{-1}(u)\phi(x)U(u)=u\phi(x), \tag{4.44}$$

so that $U(u)$ and ϕ_∞ do not commute. These superselected operators form a *non-abelian* group. Each superselected sector, as discussed earlier, can be labelled by the eigenvalues of only *one* of them.

But we want to preserve the domain $\mathscr{D}_H$ of the Hamiltonian H. The latter has a potential $V(\phi)$ which is zero only at ϕ_∞. That means that in $\mathscr{D}_H$, the operator for $\phi(x)$ must approach ϕ_∞ as $r\to\infty$. Hence, we label the superselection sector by ϕ_∞. But then $U(u)$ changes ϕ_∞ to $u\phi_\infty$ and is spontaneously broken.

It is possible to express ϕ_∞ in terms of the field ϕ smeared with a test function and its expectation value for vectors $|\cdot\rangle\in\mathscr{D}_H$.

4.10 Non-linear Models and Edge Excitations

Consider a model for Goldstone modes with gauge group G which is spontaneously broken to $H\subset G$. Then the model describes Goldstone modes with target space G/H. If the model can be described as a gauge theory, then we can apply the previous discussion. This can be done as follows [26]. We fix an orthonormal basis of the Lie algebra of G:

$$T(\alpha),\qquad \alpha=1,2,\ldots,|H|, \tag{4.45}$$

$$S(i),\qquad \text{remaining generators of } G. \tag{4.46}$$

Then under an action of $h\in H$,

$$hT(\alpha)h^{-1}=T(\beta)h_{\beta\alpha}, \tag{4.47}$$

$$hS(i)h^{-1}=S(j)D_{ji}(h). \tag{4.48}$$

Set

$$A_\mu(g) = T(\alpha)\mathrm{Tr}\, T(\alpha) g^{-1}(x)\partial_\mu g(x), \tag{4.49}$$
$$B_\mu(g) = S(i)\mathrm{Tr}\, S(i) g^{-1}(x)\partial_\mu g(x). \tag{4.50}$$

Then under the right action of H,

$$A_\mu(gh) = h^{-1}A_\mu(g)h + h^{-1}\partial_m u h, \tag{4.51}$$
$$B_\mu(gh) = h^{-1}B_\mu(g)h, \tag{4.52}$$

i.e. A_μ is a connection while B_μ is a tensor field.

For gauge group $\mathscr{H} \ni h : \mathbb{R}^n \to H$, we can write Lagrangian densities like

$$\mathscr{L}_1 = -\lambda \mathrm{Tr}\, B_\mu(g) B^\mu(g), \tag{4.53}$$

or

$$\mathscr{L}_2 = -\lambda \mathrm{Tr}\, F_{\mu\nu}(A) F^{\mu\nu}(A). \tag{4.54}$$

They reduce to standard σ-model Lagrangians, e.g. with $G = SU(2)$, $H = U(1)$, so that $G/H = S^2$. Explicitly writing:

$$g(x)\sigma_3 g^{-1}(x) = \sigma_\alpha \varphi_\alpha(x) \Rightarrow \varphi_\alpha(x)\varphi_\alpha(x) = \mathbb{1},$$

we get

$$\mathscr{L}_1 \sim -\lambda(\partial_\mu \varphi_\alpha)(\partial^\mu \varphi_\alpha),$$
$$\mathscr{L}_2 \sim -\varepsilon^{\alpha\beta\gamma}\lambda(\varphi_\alpha \partial^\mu \varphi_\beta \partial^\nu \varphi_\gamma)^2. \tag{4.55}$$

But (non-local) observables need be invariant only under

$$\mathscr{H}_\infty = \{h \in \mathscr{H} \mid h_\infty(\hat{x}) = \lim_{r\to\infty} h(r\hat{x}) = \mathbb{1}\}. \tag{4.56}$$

Can we find such observables invariant only under $\mathscr{H}_\infty$ and not under $\mathscr{H}$? Consider the Wilson line

$$W(g, x, e) = \exp \int_\infty^x d\lambda e^\mu A_\mu(g(x + \lambda e)), \tag{4.57}$$

where e^μ is a spacelike unit vector. Under gauge transformation by $h \in \mathscr{H}$,

$$W(g, x, e) \to h_\infty(\hat{x}) W(g, x, e) h^{-1}(x). \tag{4.58}$$

Hence

$$\tilde{B}_\mu(g, x, e) \equiv W(g, x, e) B_\mu(x) [W(g, x, e)]^{-1} \tag{4.59}$$

is invariant by small, but not by large gauge transformations. $\tilde{B}_\mu(g, x, e)$ is *not* a local field. $\tilde{B}_\mu(g, x, e)|x\rangle$ is a state with edge excitations. How do we see them?

Perhaps through instantons. Thus we have the θ-vacuum term

$$\frac{\theta}{32\pi^2}\int \mathrm{Tr}F(A)\wedge F(A)$$

that we can add to the action. There are also instanton solutions of $F = *F$ (for certain groups, the ADHM method works).But this topological term cannot be reduced to an integral of standard G/H-model fields. It violates CP invariance and can induce electric dipole moment. The present limit is given by

$$\theta \leq 10^{-10}.$$

Some of these ideas extend to self-dual gravity as well.

Acknowledgements The second author acknowledges financial support from the Faculty of Sciences of Universidad de los Andes through project INV-2017-51-1444.

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Chapter 5
Quantum Control at the Boundary

A. Balmaseda and J. M. Pérez-Pardo

Abstract We present a scheme for controlling the state of a quantum system by modifying the boundary conditions. This constitutes an infinite-dimensional control problem. We provide conditions for the existence of solutions of the dynamics and prove that this system is approximately controllable.

5.1 Introduction

The development of quantum technologies is of full demanding challenges. From a technological point of view there is the difficulty of manipulating coherently quantum systems made of few particles while maintaining the quantum correlations. This implies that quantum systems have to be kept under very low temperatures and interaction with them has to be performed very fast in order to avoid decoherence [4].

A basic requirement for an effective quantum information processing system, quantum sensor or simulator is the ability to control the quantum state of the system at the individual level. Geometrical control theory has provided the mathematical background to deal with quantum spin control. Khaneja et al. showed how to obtain efficient RF pulse trains for two-spin and three-spin NMR systems by finding sub-Riemannian geodesics on a quotient space of $SU(4)$ [31] and the subsequent numerical implementations [32]. We should also mention [38] for a geometric control study of quantum spin systems and [42] for an optimal control discussion of blocks of quantum algorithms (see also [12, Chaps. 5, 6] and the recent review of geometric optimal control for quantum systems in NMR by Bonnard et al. [8] and references therein). More recently a class of optimal control problems for coupled

A. Balmaseda · J. M. Pérez-Pardo
Depto. de Matemáticas, Universidad Carlos III de Madrid,
Avda. de la Universidad 30, 28911 Madrid, Leganés, Spain

J. M. Pérez-Pardo (✉)
Instituto de Ciencias Matemáticas CSIC - UAM - UC3M - UCM (ICMAT),
C/ Nicolás Cabrera 13-15, Campus de Cantoblanco, UAM, Madrid, Spain
e-mail: jmppardo@math.uc3m.es

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_5

spin systems using geometrical tools was described in [13]. A review on the current state-of-the-art on quantum optimal control can be found in [23].

However, geometric control theory and its extension to optimal control problems suffers serious drawbacks when extended to genuine infinite dimensional quantum systems. Mainly because of the intrinsic mathematical difficulties of infinite-dimensional geometry. Nevertheless, it has been applied to the finite dimensional approximations used to model the aforementioned quantum devices such as Ion Traps, NMR quantum computers and others. One of the sources of decoherence comes precisely by the neglection of the highest energy levels in order to perform the finite-dimensional approximations [20].

Only few results on controllability of linear systems are known (see for instance Beauchard et al. [5, 6], and Chambrion et al. [11] and references therein). We should also mention that alternative to geometric control theory is the use of quadrature operators in control theory, cf. [43]. There, the conventional approach is introduction of quadrature operators, and then studying and controlling the dynamics of these quadratures, for example through their Wigner functions (see for instance [2, 10, 22]).

The quantum control at the boundary (QCB) method is a radically different approach to the problem of controlling the state of a qubit. Instead of seeking the control of the quantum state by directly interacting with it using external magnetic or electric fields, the control of the state will be achieved by manipulating the boundary conditions of the system. The spectrum of a quantum system, for instance an electron moving in a box, depends on the boundary conditions imposed on it. The typical situation is to consider either Dirichlet or Neumann boundary conditions. A modification of such boundary conditions modifies the state of the system allowing for its manipulation and, eventually, its control [26]. Addressing the problem from the genuine infinite dimensional setting provides a natural way of avoiding sources of decoherence.

The QCB paradigm has been used to show how to generate entangled states in composite systems by suitable modifications of the boundary conditions [30]. The relation of QCB and topology change has been explored in [39] and recently used to describe the physical properties of systems with moving walls [16–19, 21], but in spite of its intrinsic interest some basic issues such as the QCB controllability of simple systems has never been addressed.

In developing the theory it will be shown first, by means of a suitable chosen time-dependent unitary transformation, that the variation of the boundary conditions of the system can be implemented as a time-dependent family of Hamiltonian operators, an idea that was already anticipated in [39]. The particular instance of quasi-periodic boundary conditions will be worked out explicitly and it will be shown that the system reduces to a linear system similar to those studied by Chambrion et al. [11].

This article is organised as follows. In Sect. 5.2 we review the notions of controllability in quantum systems that we will need to address the problem. The main difficulties will also be presented. In Sect. 5.3 we introduce the magnetic Laplacian.

This provides a simple model where we will be able to implement the scheme of QCB and prove controllability rigorously. Sections 5.4 and 5.5 are devoted respectively to prove the well-posedness of the dynamics in the particular system of quantum control at the boundary considered and its approximate controllability.

5.2 Control of Quantum Systems

As stated in the introduction, one of the main objectives of the research presented in this article is to show that the paradigm of quantum control at the boundary is feasible. That is, we will prove controllability, in the sense that we are going to introduce later in this section, of a quantum system by means of modifications of the boundary conditions. Before doing that, let us review briefly some important concepts of the standard theory of control.

To fix the ideas in the context of Quantum Control, cf. [12], consider the following setting. The space of pure states is given by the complex projective space , $\mathcal{P}(\mathcal{H})$, of the separable Hilbert space $\mathcal{H}$, [9, 15, 24]. In what follows we will denote the norm and scalar product of the Hilbert space by the usual notation, i.e. $\|\cdot\|$ and $\langle\cdot,\cdot\rangle$ respectively.

Evolution in a quantum system is governed in general by the time-dependent Schrödinger Equation. The final purpose of Control Theory is to study how to introduce an interaction into a system in order to be able to drive the state of the system from a given initial state to a desired target state. A simple, yet convenient, setting to define quantum control is to consider a time-dependent Hamiltonian of the form

$$H(t) = H_0 + \sum_{i=1}^{n} f_i(t) H_i \,, \tag{5.1}$$

where H_0 and H_i are self-adjoint operators on the Hilbert space and where $f_i(t) \in \mathcal{C}$ are one variable functions on a convenient space of functions. The latter has to be specified and depends on the particular problem that one wants to address. Since Control Theory is devised ultimately to be applied to some concrete experimental setting, the limitations or restrictions to be imposed on the family of controls $\mathcal{C}$ will come from the experimental setup. For simplicity let us consider for the moment that $\mathcal{C} \equiv \mathcal{C}^\infty(\mathbb{R})$, the space of smooth and real-valued functions. Given an initial state $\Psi_0 \in \mathcal{P}(\mathcal{H})$ and a target state $\Psi_T \in \mathcal{P}(\mathcal{H})$, the problem of controllability consists on determining if there exists a choice of the functions $f_i(t) \in \mathcal{C}$ such that the solution of the time-dependent Schrödinger Equation is such that the initial state Ψ_0 is driven to the target state Ψ_T in a time $T > 0$. In order to give a more precise definition of controllability let us introduce the reachable set.

Definition 1 Let $\Psi_0 \in \mathcal{P}(\mathcal{H}), f_i(t) \in \mathcal{C}, i = 1, \ldots, n$ and let $\Psi(t)$ be the solution of the time dependent Schrödinger Equation

$$i\frac{\mathrm{d}}{\mathrm{d}t}\Psi(t) = H(t)\Psi(t).$$

The **reachable set** $\mathcal{R}_{\Psi_0}(T)$ of the state Ψ_0 at time $T \in \mathbb{R}$ is defined to be

$$\mathcal{R}_{\Psi_0}(T) = \{\Psi \in \mathcal{P}(\mathcal{H}) \mid \Psi = \Psi(t), t < T \in \mathbb{R}, \Psi(0) = \Psi_0, f_i(t) \in \mathcal{C}, i = 1, \ldots, n\}.$$

That is, the reachable set of the state Ψ_0 is the set of all those states that can be accessed starting at the state Ψ_0 under all the possible evolutions described by the family of controls. We postpone until later in this section the considerations of existence of solutions of this time-dependent Schrödinger Equation. For the definition of reachable set it is implicitly assumed that the initial value problem is well-posed. We are ready now to define the notion of exact controllability.

Definition 2 Let $\mathcal{C}$ be a family of controls, let the quantum system defined by the space of states $\mathcal{P}(\mathcal{H})$ and evolution determined by the time-dependent Schrödinger Equation

$$i\frac{\mathrm{d}}{\mathrm{d}t}\Psi(t) = H(t)\Psi(t),$$

with Hamiltonian $H(t) = H_0 + \sum_{i=1}^{n} f_i(t)H_i, f_i(t) \in \mathcal{C}, i = 1, \ldots, n$. The quantum system is said to be **exactly controllable** if for all $\Psi_0 \in \mathcal{P}(\mathcal{H})$ one has that

$$\bigcup_{T\in\mathbb{R}} \mathcal{R}_{\Psi_0}(T) = \mathcal{P}(\mathcal{H}).$$

This notion is also called in the literature pure state controllability. We are only interested in the evolution of pure states $\Psi \in \mathcal{P}(\mathcal{H})$, in contrast to the more general density states.

Let us say now that the problem of controllability is a problem of existence of controls such that any target state can be achieved. The problem of (optimal) determination of the controls will not be considered here.

In general, the quantum systems are defined on infinite-dimensional Hilbert spaces. Moreover, typically the Hamiltonians are unbounded operators acting on the Hilbert space of the system. Unbounded operators are not continuous operators on the Hilbert space and therefore, existence of solutions of the time-dependent Schrödinger Equation is compromised. For instance, the domains of the operators may depend also on time, and the range of the operators may not preserve the domains. These facts introduce a set of stringent conditions on the families of available Hamiltonians, and thus of available controls, in order to define well-posed control problems. One of the aims of this article is to show that the setting of quantum control at the boundary is feasible. In particular this implies guaranteeing the existence of solutions of the evolution equation.

Quantum systems of mechanical type are governed by Hamiltonians defined by differential operators on Riemannian manifolds. Typically, the Laplace-Beltrami operator or other second order differential operator related to it. If the Riemannian manifold has boundaries those operators are in general symmetric operators but not self-adjoint, cf. [41] or [29] and references therein for an introduction to the topic. Each self-adjoint extension describes a different physical situation. Consider, for example, the case of the Laplace operator on a compact interval. One can consider Dirichlet boundary conditions or Neumann boundary conditions. These two operators define two completely different self-adjoint extensions of the same operator and thus describe completely different evolutions. The space of self-adjoint extensions of a symmetric, second order differential operator (in any dimension) can be characterised by certain families of boundary conditions, cf. [25, 27] and references therein.

We will consider the use of these spaces of boundary conditions as spaces of controls. This idea was firstly introduced in [26]. The appearance of the controls in the Hamiltonian are now more subtle than they are in (5.1) since they will not appear directly in the functional form of the operator, but will appear in the boundary conditions that define the different domains of the operators at every instant of time. That is, we are going to consider families of Hamiltonians $(H, \mathcal{D}(f_i))$, $f_i(t) \in \mathcal{C}$, where the space of controls $\mathcal{C}$ is now the space of self-adjoint extensions (or a subset of it) of the symmetric operator H.

From these previous considerations it follows that the setting of quantum control at the boundary requires of infinite-dimensional Hilbert spaces and unbounded operators. Unfortunately, the usual notions of control introduced at the beginning of this section are not suitable to handle the infinite dimensional situation. In particular, they turn out be too strict and there is the need to introduce a notion of controllability that is slightly weaker. Consider the quantum control system defined by the Harmonic oscillator over the real line

$$H_0 = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}x^2\,, \quad H_1 = x\,, \quad \mathcal{C} \equiv \mathcal{C}^\infty(t)\,,$$

such that $H(t) = H_0 + f(t)H_1, f(t) \in \mathcal{C}$. This quantum control system is not exactly controllable, see for instance [37]. However, every finite dimensional truncation up to the first n lowest eigensates, whose Hamiltonians are now given by Hermitean matrices $\tilde{H}_0$, $\tilde{H}_1 \in M(\mathbb{C})^{n\times n}$ is exactly controllable, [40]. This situation motivates the definition of approximate controllability.

Definition 3 Let $\Psi_0, \Psi_T \in \mathcal{P}(H)$. Let $B_\epsilon(\Psi_T)$ be the ball of radius $\epsilon > 0$ centred at Ψ_T. We will say that a quantum system is **approximately controllable** if for every $\epsilon > 0$ there exists a $T > 0$ such that

$$\mathcal{R}_{\Psi_0}(T) \cap B_\epsilon(\Psi_T) \neq \emptyset.$$

That is, a quantum system is approximately controllable if there is a finite time T such that the reachable set $\mathcal{R}_{\Psi_0}(T)$ of the state Ψ_0 intersects with a neighbourhood

of radius ϵ of the state Ψ_T. Therefore, one can come as close to the target state Ψ_T as desired. It is remarkable that approximate controllability has been proven , cf. [11], for linear systems with one control ($n = 1$) under suitable assumptions on the spectral properties of the operators H_0 and H_1. On Sect. 5.5 we will rely on that result to prove controllability for a particular instance of quantum control at the boundary. We should mention here that more general notions of controllability, suitable for quantum systems, are also possible, e.g. [28].

5.3 Magnetic Laplacian

During the rest of this work we will concentrate in one particular class of quantum systems, namely magnetic Laplacians in one dimension. The reason behind this choice is twofold. On one hand these systems are simple enough such that we will be able to prove rigorously the existence of dynamics and to address the boundary controllability problem. On the other hand, this simple system can be implemented physically, thus opening an interesting path to devise applications of the scheme of quantum control at the boundary to quantum computation and quantum information. Let $L \subset \mathbb{R}$ be a compact interval that for convenience we will consider to be $L = [0, l]$. The Hamiltonian of the magnetic Laplacian takes the form:

$$H = -\left(\frac{d}{dx} - iA(x)\right)^2 =: -D^2,$$

where $A \in \mathcal{H}^1(L)$ is a function in the Sobolev space of order 1 and is called the magnetic potential.

From its definition it can be seen the similarity of this Hamiltonian with the Laplace operator. This operator describes the so called *minimal coupling* of an electrically charged particle with a magnetic potential. This justifies the name of magnetic Laplacian. It is a second order differential operator and we need to determine a domain for it in order to have it well defined. Following [3, 27, 34] we will identify the domains of self-adjointness by looking for maximal domains where the boundary term of Green's formula vanishes identically. This boundary term reads in this case:

$$i\Sigma(\Phi, \Psi) := i(\langle \Psi, D^2\Phi\rangle - \langle D^2\Psi, \Phi\rangle) = \langle \underline{\Psi} + i\underline{\overset{\frown}{D\Psi}}, \underline{\Phi} + i\underline{\overset{\frown}{D\Phi}}\rangle_{\partial L}$$
$$-\langle \underline{\Psi} - i\underline{\overset{\frown}{D\Psi}}, \underline{\Phi} - i\underline{\overset{\frown}{D\Phi}}\rangle_{\partial L}.$$

The underline notation stands for restrictions to the boundary, while the arrows over the symbols mean that the restriction to the boundary is taken having into account the orientation. That is, derivatives are taken with orientation pointing outwards to the boundary as well as the restriction to the boundary of the potentials (they are one-forms evaluated on the normal vector to the boundary). The subindex ∂L means

that it is considered the scalar product of the Hilbert space induced at the boundary of L. Therefore, cf. [3], the self-adjoint extensions of D^2 are parametrized by an unitary operator $U \in \mathcal{U}(\mathcal{L}^2(\partial L))$ with

$$\operatorname{dom} D_U^2 = \{\Phi \in \mathcal{H}^2(L) : \underline{\Phi} - i\underline{\widetilde{D\Phi}} = U(\underline{\Phi} + i\underline{\widetilde{D\Phi}})\},$$

where $\mathcal{H}^2(L)$ is the Sobolev space of order 2.

It is going to be convenient for the next section to keep in mind the following well-known property about magnetic Laplacians (see, e.g., [35] for a more detailed study of this properties).

Proposition 1 *Let D_U^2 be a self-adjoint extension of the magnetic Laplacian associated to a vector potential A. Then, for any $\tilde{A}$ there exists a self-adjoint extension of the associated magnetic Laplacian, $\tilde{D}_V^2$, and an isometry T on $\mathcal{L}^2(L)$ mapping* $\operatorname{dom} \tilde{D}_V^2$ *into* $\operatorname{dom} D_U^2$ *such that*

$$T^{-1} D_U^2 T = \tilde{D}_V^2.$$

Moreover, $V = \underline{T}^{-1} U \underline{T}$ with $\underline{T}$ the restriction to the boundary of T, i.e. the operator $\underline{T} : \mathcal{L}^2(\partial L) \mapsto \mathcal{L}^2(\partial L)$ such that $\underline{T}\,\underline{\Phi} = \underline{T\Phi}$ for any $\Phi \in \mathcal{H}^2(L)$.

Proof As we already said, the magnetic vector potential is taken to be continuous and therefore, by the Poincaré Lemma, there exists $\chi : L \to \mathbb{R}$ differentiable such that $\chi' = A - \tilde{A}$. Let T denote the multiplication map defined by

$$T : \Phi \in \mathcal{L}^2(L) \mapsto e^{i\chi}\Phi \in \mathcal{L}^2(L). \tag{5.2}$$

It follows directly from this definition that T is an isometry on $\mathcal{L}^2(L)$. Using the product rule, it is easy to check that

$$\left(\frac{d}{dx} - iA(x)\right) T\Psi = T\left(\frac{d}{dx} - i\tilde{A}(x)\right)\Psi.$$

Evaluating at the boundary, it follows

$$\underline{D_U T\Psi} = \underline{T\tilde{D}_V\Psi} = \underline{T}\,\underline{\tilde{D}_V\Psi},$$

where $\underline{T}$ is the diagonal matrix $\underline{T} = \operatorname{diag}(\{e^{i\underline{\chi}(v)}\}_{v\in\partial L})$.

Using this, it is straightforward to show that for any $\Phi \in \operatorname{dom} D_U^2$, $\Psi = T^{-1}\Phi$ is in $\operatorname{dom} \tilde{D}_V^2$, if $V = \underline{T}^{-1} U \underline{T}$. Moreover,

$$D_U^2 T\Psi = T\tilde{D}^2_{\underline{T}^{-1}U\underline{T}},$$

which concludes the proof.

As a consequence of this property, we show the following result which will allow us to consider constant vector potentials.

Corollary 1 *Every self-adjoint extension of a magnetic Laplacian D_U^2, associated with a potential A, is equivalent to one associated with a constant potential $\tilde{A}$ such that* $\operatorname{dom} D_U^2 = \operatorname{dom} \tilde{D}_U^2$.

Proof Let l denote the length of the interval, i.e. $\int_L \mathrm{d}x = l$. Take $\tilde{A} = l^{-1} \int_L A(x)\,\mathrm{d}x$ and $\chi(x) = \int_0^x (A(x) - \tilde{A})\,\mathrm{d}x$. Define

$$\tilde{D}_U^2 = \left(\frac{d}{dx} - i\tilde{A}\right)^2$$

and T as in Proposition 1; it follows that $\underline{T} = \mathbb{I}_{2\times 2}$ and therefore by Proposition 1

$$T^{-1} D_U^2 T = \tilde{D}_U^2.$$

Finally, it follows straightforwardly from the previous corollary the next result, wich will be the base result for our main purpose to prove controllability at the boundary.

Corollary 2 *Let Δ stand for the Laplacian, i.e. D^2 with $A \equiv 0$. For every magnetic Laplacian, D_U^2, there is an equivalent self-adjoint extension of the Laplacian. Moreover, if T is the multiplication operator defined on (5.2) with χ such that $\chi' = A$, then*

$$T^{-1} D_U^2 T = \Delta_{\underline{T}^{-1} U \underline{T}}.$$

Among the possible unitary operators $U \in \mathcal{U}(\partial L) \simeq \mathcal{U}(\mathbb{C}^2)$ that one can consider, there are different relevant particular choices. It is important to mention that $U = \mathbb{I}_{2\times 2}$ defines Neumann boundary conditions while $U = -\mathbb{I}_{2\times 2}$ defines Dirichlet boundary conditions. A simple calculation shows that $U = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ defines periodic boundary conditions, i.e. $\Phi(0) = \Phi(l)$, $(D\Phi)(0) = (D\Phi)(l)$. The previous corollaries allow us to define the family of boundary conditions that we will use for the implementation of quantum control at the boundary.

Definition 4 Let D_U be a magnetic Laplacian on the interval L with periodic boundary conditions and with a constant magnetic potential. Let T be the multiplication operator defined by (5.2) with $\chi : L \mapsto \mathbb{R}$ such that $\frac{\mathrm{d}\chi}{\mathrm{d}x} = A$. Then $V = \underline{T}^{-1} U \underline{T}$ defines quasi-periodic boundary conditions.

A simple computation shows that the unitary operators appearing in this definition are:

$$V = \begin{bmatrix} 0 & e^{-iAl} \\ e^{iAl} & 0 \end{bmatrix}, \qquad \underline{T} = \begin{bmatrix} 1 & 0 \\ 0 & e^{iA} \end{bmatrix} e^{ib},$$

where b is the constant of integration in the definition of the function $\chi(x)$.

The way in which we are going to make use of the result in Corollary 2 is as follows. As the quantum control system we will take a free particle moving in the interval L. That is, the family of Hamiltonians is taken to be the standard Laplacian or, equivalently, the magnetic Laplacian with $A \equiv 0$. As explained earlier in this section, these operators are not well defined until we fix the corresponding domains. Each operator in this family is going to be characterised by a different quasi-periodic boundary condition. By Corollaries 1 and 2 each of these systems is unitarily equivalent to a magnetic Laplacian with constant magnetic potential A and periodic boundary conditions. We stress here that by constant we mean that the potential has the same value, independent of the point of the interval. From now on we will use the same symbol A to denote the constant magnetic potential $A \in \mathcal{H}^1(L)$ and its value $A \in \mathbb{R}$. We are going to consider that the the constant $b = 0$. The transformation T of (5.2) is defined in this case by the function

$$\chi(x) = Ax.$$

We want now to implement the scheme of quantum control at the boundary. This means that we are going to use the parameter A defining the boundary condition as our control and we will suppose that now $A = A(t)$ is a function of time. At every instant of time it will still be a constant magnetic potential along the interval L, but its magnitude will depend on time and constitute our control parameter.

Thus, we consider a quantum control system whose Hamiltonians are standard Laplacians with time-dependent quasi-periodic boundary conditions such that

$$\underline{\Psi}(0) = e^{-i\underline{\chi}(l,t)}\underline{\Psi}(l), \tag{5.3}$$

where now

$$\chi(x, t) = A(t)x \tag{5.4}$$

forms a family of functions from L to $\mathbb{R}$. One should notice that the time dependence of these Hamiltonians is subtle: usually one faces the problem where $\operatorname{dom} H(t)$ does not depend on time but the explicit, functional form of $H(t)$ does, while here we have $-\Delta$ for every t and $\operatorname{dom} \Delta$ varying with time. That is, we are considering at each time a different self-adjoint extension of the Laplacian on our interval L.

Therefore, as anticipated in the previous section, looking for solutions of the time-dependent Schrödinger equation is harder than in the most common situations. However, based on the equivalence established in this section we will be able to transform these problems into equivalent ones with Hamiltonian $H(t)$ such that $\operatorname{dom} H(t)$ remains independent of t and time dependence appears explicitly in the form of $H(t)$.

In summary, we are interested in the following control problem.

Definition 5 Consider the compact interval $L = [0, l]$. The **boundary control system associated to** L is the family of quantum Hamiltonians defined by the Laplace operator and domains given by quasi-periodic boundary conditions $\mathrm{dom}\, \Delta_{U(t)}$, with

$$U(t) = \begin{bmatrix} 0 & e^{-iA(t)l} \\ e^{iA(t)l} & 0 \end{bmatrix}.$$

5.4 Existence of Dynamics in Boundary Control Systems

The aim of this section is to study the dynamics of a boundary control system as defined in Definition 5. It will turn out that the dynamics will be well defined if the control function $A : \mathbb{R} \mapsto \mathcal{H}^1(L)$ varies smoothly with time. Quantum systems' evolution is given by a Hamiltonian operator $H(t)$, which in the most general setting depends itself on the time t, and according to Schrödinger equation

$$i\frac{\mathrm{d}}{\mathrm{d}t}\Psi(t) = H(t)\Psi(t). \tag{5.5}$$

In the case we are interested on $H(t)$ is a family of differential operators on $\mathcal{L}^2(L)$ and $\Psi(t)$ is a curve in the state space $\mathcal{P}(\mathcal{H})$.

Concerning the existence of solutions for the Schrödinger equation with a given Hamiltonian, there are several results establishing conditions for solutions to exist [33, 41]. It is customary to search for solutions using the idea of unitary propagators, which are families of operators which allow us to write the solution of the Schrödinger equation with initial state Ψ_s at $t = s$ as $\Psi(t) = U(t, s)\Psi_s$ for $t > s$. A proper definition of a unitary propagator would be as follows:

Definition 6 A two-parameter family of unitary operators $U(s, t)$, with $s, t \in \mathbb{R}$, that satisfies:

(i) $U(r, s)U(s, t) = U(r, t)$
(ii) $U(t, t) = I$
(iii) $U(s, t)$ is jointly strongly continuous in s and t

is called a **unitary propagator**.

After unitary propagators are introduced, the existence of the solutions for the associated Cauchy problems is equivalent to the existence of a unitary propagator for the (5.5). For the most general setting, in which $\mathrm{dom}\, H(t)$ varies with t, J. Kisyński gave conditions that $H(t)$ must satisfy for the unitary propagator to exist [33]. However, we will be interested in the less general case in which $\mathcal{D} = \mathrm{dom}\, H(t)$ is the same for every t and thus it is enough to consider a less general result by Reed and Simon [41, §X.12]. Instead of treating the case of families of self-adjoint operators, they study the more general case of families of generators of contraction semigroups, which can be directly applied to the case of families of self-adjoint operators since

for H self-adjoint, $\pm iH$ is the generator of a contraction semigroup (see Theorem X.47a and Example 1 on §X.8 of [41]).

Let $S(t)$ denote a family of generators of a contraction semigroup. For such a case, Reed and Simon define an approximation for the propagator $U(t, s)$ solving the equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\varphi(t) = -S(t)\varphi(t), \qquad \varphi(s) = \varphi_s$$

in the following way. First there is considered a partition of the time interval, taking a generator which is constant on each element of the partition and providing conditions ensuring that it converges to the solution. If, for example, the time interval we are interested in is $I = [0, 1]$, they take the partition made of k elements $I_j = [\frac{j-1}{k}, \frac{j}{k}]$, $1 \leq j \leq k$, and define the approximate propagator

$$U_k(t, s) = \begin{cases} \exp\left(-i(t-s)S\left(\frac{j-1}{k}\right)\right) & \text{if } \frac{j-1}{k} \leq s \leq t \leq \frac{j}{k} \\ U_k(t, \frac{j-1}{k})U_k(\frac{j-1}{k}, \frac{j-2}{k}) \ldots U_k(\frac{j-l}{k}, s) & \text{if } \frac{j-(l+1)}{k} \leq s \leq \frac{j-l}{k} \leq \frac{j-1}{k} \leq t \leq \frac{j}{k}. \end{cases} \tag{5.6}$$

That is, if s, t lie in the same interval I_j they consider the evolution operator given by the action of the contraction semigroup generated by $S(\frac{j-1}{k})$ and if t, s lie in different intervals, they use the product property of the unitary propagator to define it.

Before stating the Theorem by M. Reed and B. Simon let us prove the following result that allows to treat the boundary control problem as a time dependent problem with fixed domain. Following the ideas exposed in the previous section, we can find a natural equivalence between a boundary control system and a magnetic controlled one:

Proposition 2 *Every boundary control system is (unitarily) equivalent to a magnetic control system, that is, a system whose evolution is given by the Hamiltonian*

$$H(t) = -\left[\left(\frac{\mathrm{d}}{\mathrm{d}x} - iA(t)\right)^2 + A'(t)x\right]$$

with periodic boundary conditions and controls $A : I \subset \mathbb{R} \mapsto \mathcal{H}^1(L)$, where I is some compact interval and $\mathcal{H}^1(L)$ is the Sobolev space of order 1 on the interval L.

Proof Take the family of unitary transformations $T(t)$ as in (5.2) with $\chi = \chi(t)$:

$$T(t) : \Psi \in \mathcal{L}^2(L) \mapsto e^{i\chi(t)}\Psi \in \mathcal{L}^2(L).$$

Define $\Phi(t) = T(t)\Psi(t)$. The chain rule implies

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi(t) = \frac{\mathrm{d}T}{\mathrm{d}t}(t)\Psi(t) + T(t)\frac{\mathrm{d}}{\mathrm{d}t}\Psi(t),$$

where the derivatives of the operators have to be understood in the strong operator topology sense. Using the Schrödinger equation for Ψ, cf. (5.5), and the definition of $T(t)$, we have

$$i\frac{\mathrm{d}}{\mathrm{d}t}\Phi(t) = \left[-\frac{\mathrm{d}}{\mathrm{d}t}\chi(t) - T(t)\Delta T(t)^{-1}\right]\Phi(t).$$

Take $\chi(t) = A(t)x$ as in (5.4) and remember that we are assuming that the integration constant is $b = 0$. Thus, we have $\chi(t) = A(t)x$ and $T(t)\Delta T(t)^{-1} = -\left(\frac{\mathrm{d}}{\mathrm{d}x} - iA(t)\right)^2 =: -D^2$. Thus we have finally that

$$i\frac{\mathrm{d}}{\mathrm{d}t}\Phi(t) = -\left[\left(\frac{\mathrm{d}}{\mathrm{d}x} - iA(t)\right)^2 + A'(t)x\right]\Phi(t),$$

with periodic boundary conditions for every $t \in I$:

$$\begin{cases} \Phi(0) = \Phi(l) \\ (D\Phi)(0) = (D\Phi)(l) \Leftrightarrow \left.\frac{\mathrm{d}\Phi}{\mathrm{d}x}\right|_{x=0} = \left.\frac{\mathrm{d}\Phi}{\mathrm{d}x}\right|_{x=l}. \end{cases}$$

Notice that the equivalence in the last condition follows because we are considering magnetic potentials that are constant on the interval L. This proposition shows how to treat the boundary control system applying a unitary transformation which leads to a magnetic controlled system, where the time-dependence of the Hamiltonian's domain has been removed.

For each $t \in \mathbb{R}$ let $S(t) : \mathcal{D} \subset \mathcal{H} \mapsto \mathcal{H}$ be the generator of a contraction semigroup, densely defined on $\mathcal{D}$. Notice that we are assuming that the domain $\mathcal{D}$ remains fixed for every t. Let $\rho(S(t))$ denote the resolvent set of the operator $S(t)$ and assume that $0 \in \rho(S(t))$ for all $t \in \mathbb{R}$. For convenience of the notation it is defined a two-parameter family of operators

$$C(t, s) = S(t)S(s)^{-1} - I.$$

Note that $0 \in \rho(S(t))$ for all t implies that $S(t)$ is a bijection of $\mathcal{D}$ onto $\mathcal{H}$, and therefore $C(t, s)$ it is a bounded operator by the Closed Graph Theorem. Moreover, for every $\Phi \in \mathcal{H}$ and every $s \in \mathbb{R}$ there exists $\Psi \in \mathcal{D}$ such that $\Phi = S(s)\Psi$. Thus, for that Φ,

$$C(t, s)\Phi = S(t)\Psi - S(s)\Psi.$$

That is, studying the behaviour of $C(t, s)\Phi$ for any $\Phi \in \mathcal{H}$ can be understood as studying that of $S(t)\Psi - S(s)\Psi$ for any $\Psi \in \mathcal{D}$. In order to prove existence of dynamics of the boundary control system we are going to use the next result by M. Reed and B. Simon in what follows.

Theorem 1 (Reed and Simon [41, Thm. X.70]) *Let $\mathcal{H}$ be a Hilbert space and let I be an open interval in $\mathbb{R}$. For each $t \in I$, let $S(t)$ be the generator of a contraction semigroup on $\mathcal{H}$ so that $0 \in \rho(S(t))$ and*

(a) The $S(t)$ have common domain $\mathcal{D}$.
(b) For each $\Phi \in \mathcal{H}$, $(t-s)^{-1}C(t,s)\Phi$ is uniformly strongly continuous and uniformly bounded in s and t for $t \neq s$ lying in any fixed compact subinterval of I.
(c) For each $\Phi \in \mathcal{H}$, $C(t)\Phi = \lim_{s \nearrow t}(t-s)^{-1}C(t,s)\Phi$ exists uniformly for t in each compact subinterval of I and $C(t)$ is bounded and strongly continuous in t.

Then for all $s \leq t$ in any compact subinterval of I and any $\Phi \in \mathcal{H}$,

$$U(t,s)\Phi = \lim_{k\to\infty} U_k(t,s)\Phi$$

exists uniformly in s and t, where $U_k(t,s)$ is given by (5.6). Further, if $\Phi_s \in \mathcal{D}$, then $\Phi(t) = U(t,s)\Phi_s$ is in $\mathcal{D}$ for all t and satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi(t) = -S(t)\Phi(t), \qquad \Phi(s) = \Phi_s$$

and $\|\Phi(t)\| \leq \|\Phi_s\|$ for all $t \geq s$.

The rest of this section is devoted to prove that the family of magnetic Laplacians of Proposition 2 meets the conditions of the Theorem 1.

We are going to work with Hamiltonians whose time-dependent structure can be written as

$$H(t) = \sum_{i=1}^{n} f_i(t)H_i,$$

with $f_i : \mathbb{R} \to \mathbb{R}$ containing all the time dependence and H_i being constant symmetric operators. Applying Theorem 1 to this type of Hamiltonians is the purpose of Theorem 2, which establishes sufficient conditions to be fulfilled so that the existence of a unitary propagator is guaranteed.

Theorem 2 *Let $\{H_i\}_{i=1}^n$ be a family of symmetric operators densely defined on $\mathcal{D} \subset \mathcal{H}$ and let $f_i : I \subset \mathbb{R} \to \mathbb{R}$ be real valued functions for $1 \leq i \leq n$. Define the time-dependent operator*

$$H(t) = \sum_{i=1}^{n} f_i(t)H_i, \qquad \operatorname{dom} H(t) = \mathcal{D}.$$

If it holds

(i) $H(t)$ is self-adjoint for all $t \in I$,
(ii) $f_i \in C^1(I)$ for every i, and

(iii) for every i there exists a $K > 0$ (not depending on t) such that for every $\Psi \in \mathcal{D}$,

$$\|H_i\Psi\| \leq K(\|H(t)\Psi\| + \|\Psi\|)$$

for every $t \in I$.

Then, there exists a strongly differentiable unitary propagator $U(t,s)$ with $s,t \in I$ such that, for any $\Psi_s \in \mathcal{D}$, $\Psi(t) = U(t,s)\Psi_s$ satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\Psi(t) = -iH(t)\Psi(t), \qquad \Psi(s) = \Psi_s.$$

Before we introduce the proof it is useful to introduce the following lemmas.

Lemma 1 *Let $H(t)$ be as in Theorem 2 and define $S_i = iH_i$ and $\tilde{S}(t) = iH(t) + I$. Then, for every $\Phi \in \mathcal{H}$, there exists $K > 0$, independent of Φ and t, such that*

$$\left\| S_i \tilde{S}(t)^{-1}\Phi \right\| \leq K \|\Phi\| .$$

Proof Since $H(t)$ is self-adjoint, the spectrum of $\tilde{S}(t)$ is a subset of $i\mathbb{R} + 1 = \{i\alpha + 1 : \alpha \in \mathbb{R}\} \subset \mathbb{C}$. Thus $\tilde{S}^{-1}$ is bounded and maps $\mathcal{H}$ onto $\mathcal{D}$.

That said, this lemma is a direct consequence of hypothesis (*iii*) of Theorem 2. For every $\Psi \in \mathcal{D}$,

$$\begin{aligned}\|S_i\Psi\| = \|H_i\Psi\| &\leq K(\|H(t)\Psi\| + \|\Psi\|) \\ &= K\left(\left\|\tilde{S}(t)\Psi - \Psi\right\| + \|\Psi\|\right) \leq K\left(\left\|\tilde{S}(t)\Psi\right\| + 2\|\Psi\|\right)\end{aligned}$$

for every t. Since $\tilde{S}(t)^{-1}\Phi \in \mathcal{D}$, for every $\Phi \in \mathcal{H}$ it holds:

$$\left\| S_i \tilde{S}(t)^{-1}\Phi \right\| \leq K\left(\|\Phi\| + 2\left\|\tilde{S}(t)^{-1}\Phi\right\|\right).$$

The distance from 0 to $\sigma(\tilde{S}(t))$ is at least 1, and thus $\left\|\tilde{S}(t)^{-1}\right\| \leq 1$. Hence, renaming the constant we get

$$\left\| S_i \tilde{S}(t)^{-1}\Phi \right\| \leq K \|\Phi\| .$$

Lemma 2 *Let $H(t)$ be as in Theorem 2 and define $S_i = iH_i$ and $\tilde{S}(t) = iH(t) + I$. Then, for s, t lying in a compact subset of I and for every $\Phi \in \mathcal{H}$, $\lim_{t\to s} \tilde{S}(t)\tilde{S}(s)^{-1}\Phi = \Phi$ uniformly on s.*

Proof We need to prove the limit uniformly on s, i.e., that

$$\lim_{t\to s} \left\| \tilde{S}(t)\tilde{S}(s)^{-1}\Phi - \Phi \right\| = 0$$

uniformly on s. We have

$$\left\|\tilde{S}(t)\tilde{S}(s)^{-1}\Phi-\Phi\right\| = \left\|\sum_{i=1}^{n}[f_i(t)-f_i(s)]S_i\tilde{S}(s)^{-1}\Phi\right\| \leq \sum_{i=1}^{n}|f_i(t)-f_i(s)|\left\|S_i\tilde{S}(s)^{-1}\Phi\right\|.$$

Now, using Lemma 1 one gets

$$\left\|\tilde{S}(t)\tilde{S}(s)^{-1}\Phi-\Phi\right\| \leq K\sum_{i=1}^{n}|f_i(t)-f_i(s)|\,\|\Phi\|.$$

Hence, $\lim_{t\to s}\left\|\tilde{S}(t)\tilde{S}(s)^{-1}\Phi-\Phi\right\|=0$ uniformly on s since every f_i is uniformly continuous on I (which follows from (*ii*) and the fact that we are considering a fixed, compact subset of I).

Proof (*Proof of Theorem 2*) This theorem is a consequence of Theorem 1 and the fact that $S(t)=iH(t)$ is the generator of a contraction semigroup by Hille–Yoshida theorem (see [41], Theorem X.47a and Example 1 on §X.8). In order to apply Theorem 1 we need to have $0\in\rho(iH(t))$ for every t, which is not satisfied in general. However, since $H(t)$ is self-adjoint $i\in\rho(H(t))$ for every t and therefore $-1\in\rho(S(t))$ which implies $\tilde{S}=S(t)+I$ has 0 in its resolvent set. Note that if $\Phi(t)=\tilde{U}(t,s)\xi$ satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi(t)=-\tilde{S}(t)\Phi(t),\qquad \Phi(s)=\xi,$$

then $\Psi(t)=U(t,s)\xi$ with $U(t,s):=\tilde{U}(t,s)e^{-i(s-t)}$ satisfies, by the product rule,

$$\frac{\mathrm{d}}{\mathrm{d}t}\Psi(t)=-S(t)\Psi(t),\qquad \Psi(s)=\xi.$$

Thus, existence of $\tilde{U}(t,s)$ with the properties in the statement of Theorem 2 guarantee the existence of $U(t,s)$ with the same properties.

Hence, it is enough to show that $\tilde{S}(t)$ satisfies the hypothesis of Theorem 1. It is clear that $\tilde{S}(t)$ can be written as

$$\tilde{S}(t)=I+i\sum_{j=1}^{n}f_j(t)H_j=\sum_{j=1}^{n+1}f_j(t)S_j$$

with $S_i=iH_j$, $f_{n+1}=1$ and $S_{n+1}=I$. Also is easy to check using Hille–Yoshida theorem that $\tilde{S}(t)$ is the generator of a contraction semigroup.

Hypothesis (a) of Theorem 1 is satisfied since, by definition, every $H(t)$ (and therefore $\tilde{S}(t)$) has the same domain $\mathcal{D}$.

Regarding (b) and (c), it is useful to write

$$(t-s)^{-1}C(t,s) = (t-s)^{-1}[\tilde{S}(t) - \tilde{S}(s)]\tilde{S}(s)^{-1} = \sum_{i=1}^{n} \frac{f_i(t) - f_i(s)}{t-s} S_i \tilde{S}(s)^{-1}. \tag{5.7}$$

For convenience, let us denote $g_i(t,s) = \frac{f_i(t)-f_i(s)}{t-s}$, which clearly is C^1 in s and t for $t \neq s$ in I. Moreover, for $s \neq t$ lying in any fixed compact subinterval of I, g_i is uniformly continuous because $f_i(t)$ is $C^1(I)$.

From the previous equation it follows that for $\Phi \in \mathcal{H}$

$$\left\| (t-s)^{-1}C(t,s)\Phi \right\| \leq \sum_{i=1}^{n+1} |g_i(t,s)| \left\| S_i \tilde{S}(s)^{-1}\Phi \right\| \leq K \sum_{i=1}^{n+1} |g_i(t,s)| \, \|\Phi\| ,$$

where we have used Lemma 1 in the last inequality. For $s \neq t$ lying in any fixed compact subinterval of I, $|g_i(t,s)|$ is bounded uniformly on s and t since it is continuous and thus $\left\| (t-s)^{-1}C(t,s)\Phi \right\|$ is uniformly bounded for such s, t.

For the uniform strong continuity with respect to t, it is clear that

$$\begin{aligned} \left\| (t_0-s)^{-1}C(t_0,s)\Phi - (t-s)^{-1}C(t,s)\Phi \right\| &\leq \sum_{i=1}^{n+1} |g_i(t_0,s) - g_i(t,s)| \left\| S_i \tilde{S}(s)^{-1}\Phi \right\| \\ &\leq K \sum_{i=1}^{n+1} |g_i(t_0,s) - g_i(t,s)| \, \|\Phi\| \end{aligned}$$

and, thus, uniform continuity of $t \mapsto g_i(t,s)$ implies uniform strong continuity of the operator-valued function $t \mapsto (t-s)^{-1}C(t,s)$.

On the other hand, regarding uniform strong continuity respect to s we have

$$\begin{aligned} &\left\| (t-s_0)^{-1}C(t,s_0)\Phi - (t-s)^{-1}C(t,s)\Phi \right\| \\ &\leq \sum_{i=1}^{n+1} \left\| g_i(t,s_0) S_i \tilde{S}(s_0)^{-1}\Phi - g_i(t,s) S_i \tilde{S}(s)^{-1}\Phi \right\| \\ &\leq \sum_{i=1}^{n+1} |g_i(t,s_0)| \left\| S_i \tilde{S}(s_0)^{-1}\Phi - S_i \tilde{S}(s)^{-1}\Phi \right\| + \\ &+ \sum_{i=1}^{n+1} |g_i(t,s_0) - g_i(t,s)| \left\| S_i \tilde{S}(s)^{-1}\Phi \right\| . \end{aligned} \tag{5.8}$$

Let us examine separately the two terms on the right-hand side. First,

$$\sum_{i=1}^{n+1} |g_i(t,s_0) - g_i(t,s)| \left\| S_i \tilde{S}(s)^{-1} \Phi \right\| \leq K \sum_{i=1}^{n+1} |g_i(t,s_0) - g_i(t,s)| \, \|\Phi\|$$

and therefore because g_i is uniformly continuous for $s \neq t$ in a compact subinterval of I, for every $s \neq t$ and every $\varepsilon > 0$ there exists $\delta_1 > 0$ such that for $|s_0 - s| < \delta_1$ it holds

$$\sum_{i=1}^{n+1} |g_i(t,s_0) - g_i(t,s)| \left\| S_i \tilde{S}(s)^{-1} \Phi \right\| \leq \frac{\varepsilon}{2}.$$

For the first term in (5.8),

$$\sum_{i=1}^{n+1} |g_i(t,s_0)| \left\| S_i \tilde{S}(s_0)^{-1} \Phi - S_i \tilde{S}(s)^{-1} \Phi \right\| \leq K \sum_{i=1}^{n+1} |g_i(t,s_0)| \left\| \tilde{S}(s) \tilde{S}(s_0)^{-1} \Phi - \Phi \right\|$$

and thus by Lemma 2 and the fact that g_i is uniformly bounded for $s \neq t$, for every $s \neq t$ and every $\varepsilon > 0$ there exists $\delta_2 > 0$ such that for $|s_0 - s| < \delta_2$ it holds

$$\sum_{i=1}^{n+1} |g_i(t,s_0)| \left\| S_i \tilde{S}(s_0)^{-1} \Phi - S_i \tilde{S}(s)^{-1} \Phi \right\| \leq \frac{\varepsilon}{2}.$$

Hence, taking $\delta = \min\{\delta_1, \delta_2\}$ and substituting into (5.8) we have that for $|s_0 - s| < \delta$

$$\left\| (t-s_0)^{-1} C(t,s_0) \Phi - (t-s)^{-1} C(t,s) \Phi \right\| \leq \varepsilon$$

which shows that hypothesis (b) is fulfilled.

Regarding hypothesis (c) of Theorem 1, it is easy to see that $C(t)\Phi = \sum_{i=1}^{n+1} f_i'(t) S_i \tilde{S}(t)^{-1} \Phi$. Indeed, from (5.7) we get

$$\begin{aligned}
&\left\| (t-s)^{-1} C(t,s) \Phi - \sum_{i=1}^{n+1} f_i'(t) S_i \tilde{S}(t)^{-1} \Phi \right\| \\
&= \left\| \sum_{i=1}^{n+1} \left[g_i(t,s) S_i \tilde{S}(s)^{-1} - f_i'(t) S_i \tilde{S}(t)^{-1} \right] \Phi \right\| \\
&\leq \sum_{i=1}^{n+1} |f_i'(t)| \left\| S_i \tilde{S}(s)^{-1} \Phi - S_i \tilde{S}(t)^{-1} \Phi \right\| \\
&+ \sum_{i=1}^{n+1} |g_i(t,s) - f_i'(t)| \left\| S_i \tilde{S}(s)^{-1} \Phi \right\|.
\end{aligned}$$

Using again Lemmas 1 and 2 and the fact that we are considering a compact subinterval, the continuity of every f_i' and the definition of derivative implies the limit $C(t)\Phi = \lim_{s\to t}(t-s)^{-1}C(t,s)\Phi$ exists uniformly on t and is equal to $C(t)\Phi$.

Boundedness of $C(t)$ as an operator follows directly from Lemma 1 and the continuity of $f_i'(t)$:

$$\begin{aligned}\|C(t)\Phi\| &= \left\|\sum_{i=1}^{n+1} f_i'(t) S_i \tilde{S}(t)^{-1}\Phi\right\| \leq \sum_{i=1}^{n+1} |f_i'(t)| \left\|S_i\tilde{S}(t)^{-1}\Phi\right\| \\ &\leq 2K\sum_{i=1}^{n+1}|f_i'(t)|\,\|\Phi\|\,.\end{aligned}$$

Besides existence of unitary propagators for Schrödinger equations associated with Hamiltonians of the type we are dealing with, we are going to need a result on how close the evolution induced by two of these Hamiltonians is when they are similar (in the precise sense introduced in Theorem 3).

Theorem 3 *Let H_i be symmetric operators with common domain $\mathcal{D}$. Let $f_i, g_i \in C^1(I)$, $i = 1,\dots,n$ and $I \subset \mathbb{R}$. Suppose that $H_1(t) = \sum_{i=1}^n f_i(t)H_i$ and $H_2(t) = \sum_{i=1}^n g_i(t)H_i$, with common domain $\mathcal{D}$ are self-adjoint operators, satisfying the hypothesis of Theorem 2. Then, for every $\Psi \in \mathcal{D}$, every $T > 0$ and every $\varepsilon > 0$ there exist $\delta > 0$ such that $\|f_i - g_i\|_\infty < \delta$ implies $\|U_1(T,s)\Psi - U_2(T,s)\Psi\| < \varepsilon$.*

Proof By Theorem 2, there exist unitary propagators $U_1(t,s)$, $U_2(t,s)$ associated with $H_1(t)$, $H_2(t)$ respectively. Since for any $\Psi \in \mathcal{D}$, $t \mapsto U_\ell(t,s)\Psi$ is strongly differentiable ($\ell = 1, 2$), we have $t \mapsto \|U_1(t,s)\Psi - U_2(t,s)\Psi\|$ is differentiable and by the Fundamental Theorem of Calculus we have

$$\|U_1(T,s)\Psi - U_2(T,s)\Psi\| = \int_s^T \frac{\mathrm{d}}{\mathrm{d}t}\|U_1(t,s)\Psi - U_2(t,s)\Psi\|\,\mathrm{d}t.$$

Strong differentiability implies that we can take the derivative into the norm and get

$$\begin{aligned}\|U_1(T,s)\Psi - U_2(T,s)\Psi\| &= \int_s^T \left\|\frac{\mathrm{d}}{\mathrm{d}t}U_1(t,s)\Psi - \frac{\mathrm{d}}{\mathrm{d}t}U_2(t,s)\Psi\right\|\mathrm{d}t \\ &= \int_s^T \|H_1(t)\Psi - H_2(t)\Psi\|\,\mathrm{d}t \\ &\leq \sum_{i=1}^n \int_s^T |f_i - g_i|\,\|H_i\Psi\|\,\mathrm{d}t \\ &\leq (T-s)\sum_{i=1}^n \|f_i - g_i\|_\infty \|H_i\Psi\|\end{aligned}$$

Hence, it is enough to take

$$\delta = \inf_i \frac{\varepsilon}{n(T-s)\,\|H_i\Psi\|}.$$

5.5 Approximate Controllability of Boundary Control Systems

Approximate controllability of the boundary control system is, by Proposition 2, equivalent to approximate controllability of a quantum system with Hamiltonian

$$H(t) = -\left[\left(\frac{\mathrm{d}}{\mathrm{d}x} - iA(t)\right)^2 + A'(t)x\right]$$

and periodic boundary conditions.

Unlike control on a finite dimensional Hilbert space, control on an infinite dimensional Hilbert space has no general result giving necessary and sufficient conditions for (approximate) controllability. However, it will be enough for us to rely on a theorem by Chambrion et al. [11], giving sufficient conditions to prove approximate controllability for the boundary control system. In the referenced work it is studied the approximate controllability of some linear control systems; that is, systems whose evolution is given by

$$i\frac{\mathrm{d}}{\mathrm{d}t}\Psi(t) = H_0\Psi(t) + u(t)H_1\Psi(t), \tag{5.9}$$

with $u : \mathbb{R} \to (0, c)$. Moreover, they assume that:

(A1) H_0, H_1 are self-adjoint operators not depending on t,
(A2) there exists an orthonormal basis $\{\phi_n\}_{n\in\mathbb{N}}$ of $\mathcal{H}$ made of eigenvectors of H_0, and
(A3) $\phi_n \in \operatorname{dom} H_1$ for every $n \in \mathbb{N}$.

Control systems satisfying conditions *(A1)*–*(A3)* will be called **normal quantum control systems**. For them, the following theorem is proven:

Theorem 4 (Chambrion et al. [11, Thm. 2.4]) *Consider a normal quantum control system, with $c > 0$ as described above. Let $\{\lambda_n\}_{n\in\mathbb{N}}$ denote the eigenvalues of H_0, each of them associated to the eigenfunction ϕ_n. Then, if the elements of the sequence $\{\lambda_{n+1} - \lambda_n\}_{n\in\mathbb{N}}$ are $\mathbb{Q}$-linearly independent and if $\langle\phi_{n+1}, H_1\phi_n\rangle \neq 0$ for every $n \in \mathbb{N}$, the system is approximately controllable.*

Based on this theorem we will prove the main result of this work which ensures the approximate controllability of the boundary control systems. This is the first instance in which controllability of a system using boundary controls is considered. Before doing that it is convenient to introduce the following lemma:

Lemma 3 *Consider a normal quantum control system* $i\frac{\mathrm{d}}{\mathrm{d}t}\Psi = H_0\Psi + u(t)H_1\Psi$ *with* H_0, H_1 *such that* $H(t) = H_0 + u(t)H_1$ *satisfies hypothesis of Theorem 2. Then given any* $\varepsilon > 0$ *there exist perturbed Hamiltonians* $\tilde{H}_0$, $\tilde{H}_1$ *with the same domain as* H_0 *such that they satisfy the conditions of Theorem 2 and also those of Theorem 4 and such that for every* $t > s$ *and every* C^1 *piecewise function* $u : [s, t] \to \mathbb{R}$, *it holds:*

$$\left\| U(t,s)\Psi - \tilde{U}(t,s)\Psi \right\| < \varepsilon, \qquad (\forall \Psi \in \operatorname{dom} H_0),$$

where we denote by $U(t, s)$ *and* $\tilde{U}(t, s)$ *the unitary propagators associated with* $H(t)$ *and* $\tilde{H}(t) = \tilde{H}_0 + u(t)\tilde{H}_1$ *respectively.*

Proof Let λ_k, ϕ_k denote the eigenpairs of H_0. If it is the case that $\mathbb{Q}$-linear independence condition of Theorem 4 hold, we set $\tilde{H}_0 = H_0$; otherwise take an increasing sequence of positive irrational numbers ν_k such that they are rationally independent and $\nu_k < 2^{-k}$. Then define

$$H_{0,p} = \sum_{k\in\mathbb{N}} \nu_k \phi_k \phi_k^\dagger.$$

Obviously $H_{0,p}$ has the same domain as H_0 because $\left\|H_{0,p}\Psi\right\|^2 \leq \sum_k 2^{-2k}|\langle\phi_k, \Psi\rangle|^2$, from what we get $\left\|H_{0,p}\Psi\right\| \leq \|\Psi\|$ and $H_{0,p}$ can be chosen to have the same domain as H_0.

Define $\tilde{H}_0 = H_0 + \mu_0 H_{0,p}$ with $\mu_0 \in \mathbb{Q}$. Then $\tilde{H}_0$ has eigenvalues $\lambda_k + \mu_0\nu_k$ satisfying the rationally independence condition of Theorem 4.

If H_1 is such that $\langle\phi_{n+1}, H_1\phi_n\rangle = 0$ for $n \in N \subset \mathbb{N}$, take a sequence of positive, non-vanishing terms $\{\alpha_n\}_{n\in N}$ such that $\alpha_n < 2^{-n}$ and define

$$H_{1,p} = \sum_{n\in N} \alpha_n \phi_{n+1}\phi_n^\dagger.$$

Again the domain of $H_{1,p}$ can be chosen to be dom H_0, since $\left\|H_{1,p}\Psi\right\|^2 \leq \sum_{n\in N} 2^{-2n}$ $|\langle\phi_n, \Psi\rangle|^2$ and thus $\left\|H_{1,p}\Psi\right\| \leq \|\Psi\|$.

Defining $\tilde{H}_1 = H_1 + \mu_1 H_{1,p}$ with μ_1 real it is clear that $\tilde{H}_1$ satisfies $\langle\phi_{n+1}, \tilde{H}_1\phi_n\rangle \neq 0$ for any $n \in \mathbb{N}$.

From what we already said, taking into account that $H_{0,p}$ and $H_{1,p}$ are bounded, it follows that if $H(t)$ satisfies the hypothesis of Theorem 3, so does $\tilde{H}(t)$ on each interval in which $u(\tau)$ is C^1 and therefore, taking μ_0 and μ_1 small enough we have

$$\left\| U(t,s)\Psi - \tilde{U}(t,s)\Psi \right\| < \varepsilon, \qquad \text{for all } \Psi \in \operatorname{dom} H_0.$$

Suppose that $A \in C^2(I)$ defines the time dependent magnetic vector potential. Then $H(t)$ fulfills all the hypothesis of Theorem 2 but (*iii*), which requires some work to prove. The following lemma shows that the families of Hamiltonians $H(t)$ that we consider, i.e., those on Proposition 2, satisfy hypothesis (*iii*) of Theorem 2 and therefore have well defined evolutions.

Lemma 4 *Let $A : L \to \mathbb{R}$ be a constant magnetic vector potential, and denote by $-D_A^2$ a self-adjoint extension of the associated magnetic Laplacian, whose domain we denote by $\mathcal{D} \subset \mathcal{H}^2(L)$. Let $r > 0$, and suppose that $|A| < r$. Then there exists a constant K (not depending on A) such that*

$$\left\| \frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} \right\| \leq K \left(\left\| D_A^2 \Psi \right\| + \|\Psi\| \right)$$

for all $\Psi \in \mathcal{D}$.

Proof We will prove this lemma in three steps. First, we will show that for every constant vector potential $A \in \mathcal{H}^1(L)$ the bound in the lemma stands with constant K_A depending on A. In fact, since the magnetic Laplacian is self-adjoint, $-D_A^2 + iI$ is invertible with bounded inverse and maps $\mathcal{H}$ onto $\mathcal{D} \subset \mathcal{H}^2(L)$. Also $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ is closed in $\mathcal{H}^2(L)$ since it is the adjoint of the standard Laplacian with the minimal symmetric domain (*i.e.*, with domain $\mathcal{D}_0 = \{\Psi \in \mathcal{H}^2(L) \mid \underline{\Psi} = 0, \underline{\frac{\mathrm{d}\Psi}{\mathrm{d}x}} = 0\}$) as is well-known (see, e.g., [36]). By the Closed Graph Theorem this implies that

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}(D_A^2 + iI)^{-1}$$

is a bounded operator on $\mathcal{L}^2(L)$. Therefore, for any $\Psi \in \mathcal{D}$,

$$\left\| \frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} \right\| = \left\| \frac{\mathrm{d}^2}{\mathrm{d}x^2}(D_A^2 + iI)^{-1}(D_A^2 + iI)\Psi \right\| \leq K_A \left\| (D_A^2 + iI)\Psi \right\| \leq K_A \left(\left\| D_A^2 \Psi \right\| + \|\Psi\| \right) \tag{5.10}$$

where we have defined $K_A = \left\| \frac{\mathrm{d}^2}{\mathrm{d}x^2}(D_A^2 + iI)^{-1} \right\|$.

Once we have proved (5.10), we can prove that for every constant vector potential A there exists an $\varepsilon_A > 0$ such that for any constant magnetic vector potential B satisfying $|A - B| \leq \varepsilon_A$ it holds

$$\left\| \frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} \right\| \leq \tilde{K}_A \left(\left\| D_B^2 \Psi \right\| + \|\Psi\| \right),$$

with $\tilde{K}_A > 0$ not depending on B. Indeed, from (5.10) we have

$$\left\| \frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} \right\| \leq K_A \left(\left\| D_A^2 \Psi \right\| + \|\Psi\| \right) \leq K_A \left(\left\| D_A^2 \Psi - D_B^2 \Psi \right\| + \left\| D_B^2 \Psi \right\| + \|\Psi\| \right). \tag{5.11}$$

Let us examine the first term in the parenthesis. By the definition of the Magnetic Laplacians,

$$\left\| D_A^2 \Psi - D_B^2 \Psi \right\| = \left\| (A^2 - B^2)\Psi + 2i(A - B)\frac{\mathrm{d}\Psi}{\mathrm{d}x} \right\|. \tag{5.12}$$

Denoting $\varepsilon = |A - B|$ and using the triangle inequality one gets

$$\left\| (A^2 - B^2)\Psi + 2i(A - B)\frac{\mathrm{d}\Psi}{\mathrm{d}x} \right\| \leq \varepsilon(2|A| + \varepsilon)\,\|\Psi\| + 2\varepsilon \left\| \frac{\mathrm{d}\Psi}{\mathrm{d}x} \right\|. \tag{5.13}$$

Now, using the well-known fact [1, Thm. 5.2] that

$$\left\| \frac{\mathrm{d}\Psi}{\mathrm{d}x} \right\| \leq \tilde{K} \left(\left\| \frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} \right\| + \|\Psi\| \right),$$

we get

$$\left\| (A^2 - B^2)\Psi + 2i(A - B)\frac{\mathrm{d}\Psi}{\mathrm{d}x} \right\| \leq \varepsilon(2|A| + \varepsilon + 2\tilde{K}) \left(\|\Psi\| + \left\| \frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} \right\| \right). \tag{5.14}$$

Let us define the function $\kappa(\varepsilon) := \varepsilon(2|A| + \varepsilon + 2\tilde{K})$, which is a continuous monotone function of ε with range $[0, \infty)$. Substituting back into into (5.12) we get

$$\left\| D_A^2\Psi - D_B^2\Psi \right\| \leq \kappa(\varepsilon) \left(\|\Psi\| + \left\| \frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} \right\| \right).$$

Hence, from (5.11) we have that

$$(1 - \kappa(\varepsilon)K_A) \left\| \frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} \right\| \leq K_A\,(1 + \kappa(\varepsilon)) \left(\left\| D_B^2\Psi \right\| + \|\Psi\| \right).$$

Obviously we can choose ε_A such that $\kappa(\varepsilon_A)K_A = 1/2$, and then

$$\left\| \frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} \right\| \leq 2K_A\,(1 + \kappa(\varepsilon_A)) \left(\left\| D_B^2\Psi \right\| + \|\Psi\| \right) =: \tilde{K}_A \left(\left\| D_B^2\Psi \right\| + \|\Psi\| \right).$$

The proof can be finished by a compacity argument. Since we are only considering constant vector potentials, each potential A defines a point in $\mathbb{R}$. The subset $\mathcal{K}$ of $\mathbb{R}$ associated to the set of vector potentials satisfying $|A| \leq r$ is a compact subset. Now, define $U_A = \{B \in \mathbb{R} \mid |B - A| < \varepsilon_A\}$; the family $\{U_A\}_{A \in U}$ forms a covering of $\mathcal{K}$ and by compacity it admits a finite subcovering $\{U_{A_i}\}_i$. Taking the maximum of the associated constants,

$$K = \max_i \tilde{K}_{A_i},$$

concludes the proof.

Theorem 5 *Let $\mathcal{C}_p(0, T)$ the set of piecewise two times continuously differentiable functions on the interval $[0, T]$. The boundary control system with controls $\mathcal{C}_p(0, T)$ is approximately controllable.*

Proof By Proposition 2 the boundary control system is controllable if and only if so is the magnetic controlled system given by

$$H(t) = -\left[\left(\frac{\mathrm{d}}{\mathrm{d}x} - iA(t)\right)^2 + A'(t)x\right] \tag{5.15}$$

and periodic boundary conditions. We will proof that this equivalent system is approximately controllable using Theorem 4. The main problem to do this is the fact that $A(t)$ and $A'(t)$ are not independent, and to avoid this problem we need to proceed in two steps. First we define an auxiliary system to which Theorem 4 applies and then we use Theorem 3 to show that for any controls on the auxiliary system, its evolution is approximately the same as the evolution of the original system with some controls related to those on the auxiliary system.

Let us start with the first step. Take a constant magnetic vector potential $a \in \mathcal{H}^1(L)$ with associated magnetic Laplacian $-D^2 = -\left(\frac{\mathrm{d}}{\mathrm{d}x} - ia\right)^2$. We consider

$$A'(t) = u(t), \tag{5.16}$$

where $u : I \to \mathbb{R}$ is a control, and define the auxiliary system with Hamiltonian

$$\tilde{H}(t) = -D^2 - u(t)x, \tag{5.17}$$

It is easy to check that the assumptions made by Chambrion et al. are satisfied in our case: $H_0 = -D^2$ and $H_1 = x$ are self-adjoint operators not depending on t, there exists an orthonormal basis of the Hilbert space $\mathcal{H}$ made of eigenfunctions of any magnetic Laplacian over L provided that L is compact [7, Thm. 3.1.1], and H_1 is a self-adjoint bounded operator (since L is compact) and thus $\operatorname{dom} H_1 = \mathcal{H}$.

By Lemma 3, Theorem 4 can be applied (either to $\tilde{H}(t)$ or to a perturbed system with evolution as *closed* as desired) and so the system is approximately controllable. Hence, for every initial state Ψ_0, every target state Ψ_T, every $\varepsilon > 0$ and every $c > 0$ there exists $T > 0$ and $u(t) : [0, T] \to (0, c)$ piecewise constant such that the evolution induced by $\tilde{H}(t)$ and denoted $\tilde{\Psi}(t)$, satisfies $\tilde{\Psi}(0) = \Psi_0$ and $\left\|\tilde{\Psi}(T) - \Psi_T\right\| < \varepsilon/2$. Denote by $\tilde{U}(t, s)$ the unitary propagator associated to $\tilde{H}$ with controls $u(t)$.

Now, choosing the vector potential from the original system (5.15) in such a way that its induced evolution is close enough to that of the auxiliary system, one guarantees that the evolved state reaches near the target state at time T. In order to do that, we split the time interval $[0, T]$ into N pieces of length $\tau = T/N$, and for each of those subintervals define $A_k : [k\tau, (k+1)\tau) \to \mathbb{R}$ as

$$A_k(t) = a + \int_{k\tau}^{t} u(s)\, ds,$$

with $u(t)$ the piecewise control given by Chambrion et al.'s theorem. Taking

$$A(t) = \sum_{k=0}^{N-1} \chi_{[k\tau,(k+1)\tau)}(t) A_k(t),$$

it is clear that $A'(t) = u(t)$ and therefore $A \in \mathcal{C}_p(0, T)$. Also, by the mean value theorem,

$$\|A - a\|_\infty = \max_{k<N} \sup_{k\tau \le t < (k+1)\tau} \int_{k\tau}^{t} u(s)\, ds \le c\tau \tag{5.18}$$

For the moment, τ is arbitrary but later on we will need to choose it small enough.

Expanding the square on (5.15) and having into account Lemma 4, it is easy to check that the Hamiltonian of the original system, $H(t)$, fulfills the hypothesis of Theorem 2 in every interval $[k\tau, (k+1)\tau)$.

Hence, there exists a unitary propagator $U_k(t, s)$ describing the evolution induced by it for $t, s \in [k\tau, (k+1)\tau)$. For $t \in [k\tau, (k+1)\tau]$, $s \in [\ell\tau, (\ell+1)\tau)$ with $\ell < k$ the unitary propagator is constructed multiplying them:

$$U(t, s) = U_k(t, k\tau) U_{k-1}(k\tau, (k-1)\tau) \dots U_\ell((\ell+1)\tau, s).$$

In what follows we omit the subscript on U_k since the values of its arguments t, s identify the index k unambiguously.

Finally, let $\{I_j\}$ with $I_j = [t_j, t_{j-1})$ be the coarser partition of $[0, T]$ which is a common refinement of both the partition $\{[k\tau, (k+1)\tau)\}_k$ and that given by the piecewise definition of $u(t)$. Remember that Theorem 4 proves approximate controllability for $u(t)$ piecewise-constant control functions. It is clear that the state of the system at time $T \in I_n$, assumed the evolution induced by $H(t)$ (defined in Equation (5.15)) starting at Ψ_0, can be written as

$$\Psi(T) = U(T, t_n) U(t_n, t_{n-1}) \dots U(t_1, 0) \Psi_0.$$

And similarly for the state $\tilde{\Psi}(T)$ if we assume evolution by $\tilde{H}$ defined in Equation (5.17) (using the unitary propagator $\tilde{U}$ instead of U).

It is straightforward to check that in every I_j both Hamiltonians satisfy the hypothesis of Theorem 3: the domain of magnetic Laplacians is fixed by periodic boundary conditions independent of t, and the multiplication operator x is bounded. Remember that $u(t)$ being $C^1(I_j)$, in fact constant on I_j, implies that the functions giving the time dependence of the Hamiltonians (after expanding the magnetic Laplacians) are also $C^1(I_j)$. Both Hamiltonians satisfy the hypothesis of Theorem 2 (see Lemma 4). Hence, for any $t, s \in I_j$, and any $\varepsilon_2 > 0$ we can chose $\delta = c\tau$ as in Theorem 3 so that

$$\left\| \tilde{U}(t, s)\Psi_0 - U(t, s)\Psi_0 \right\| < \varepsilon_2.$$

Hence, we have

$$\begin{aligned}\left\|\tilde{\Psi}(T)-\Psi(T)\right\| &= \left\|\tilde{U}(T,t_n)\dots\tilde{U}(t_1,s)\Psi_0 - U(T,t_n)\dots U(t_1,s)\Psi_0\right\| \\ &\leq \left\|\tilde{U}(T,t_n)\dots\tilde{U}(t_2,t_1)U(t_1,s)\Psi_0 - U(T,t_n)\dots U(t_1,s)\Psi_0\right\| + \varepsilon_2 \\ &\vdots \\ &\leq (n+1)\varepsilon_2.\end{aligned}$$

Taking $\varepsilon_2 = \varepsilon/(2n+2)$, we have

$$\left\|\tilde{\Psi}(T)-\Psi(T)\right\| \leq \frac{\varepsilon}{2}.$$

Using that for the auxiliary system we have that $\left\|\tilde{\Psi}(T)-\Psi_T\right\| < \frac{\varepsilon}{2}$, we conclude

$$\|\Psi(T)-\Psi_T\| < \varepsilon.$$

Hence, we have found a control $A:[0,T]\to\mathbb{R}$ piecewise two times continuously differentiable such that from any Ψ_0 we can reach as close as we want to any Ψ_T and so the system is approximately controllable.

Using Theorem 5 and an approximating argument similar to that in its proof, is easy to show that controls can also be smooth functions of time.

Corollary 3 *Every boundary control system with smooth controls $A:[0,T]\to\mathbb{R}$ is approximately controllable.*

Proof By Proposition 2 the boundary control system is approximately controllable if and only if so is the magnetic controlled system with

$$H(t) = -\left[\left(\frac{\mathrm{d}}{\mathrm{d}x} - iA(t)\right)^2 + A'(t)x\right]$$

and periodic boundary conditions.

From Theorem 5, for every initial state Ψ_0, every target state Ψ_T and every $\varepsilon>0$, we have piecewise two times continuously differentiable controls $\tilde{A}(t)$ such that the evolution $\tilde{\Psi}(t)$ induced by

$$\tilde{H}(t) = -\left[\left(\frac{\mathrm{d}}{\mathrm{d}x} - i\tilde{A}(t)\right)^2 + \tilde{A}'(t)x\right],$$

satisfies $\tilde{\Psi}(0)=\Psi_0$ and $\|\tilde{\Psi}(T)-\Psi_T\|<\varepsilon/2$. Denote by $\tilde{U}(t,s)$ the unitary propagator associated to $\tilde{H}(t)$.

Using some well-known approximation result (see, for example, [14, §5.3]) one can find $A(t)$ smooth such that $\left\|A - \tilde{A}\right\| < \delta_1$ and $\left\|A' - \tilde{A}'\right\| < \delta_2$. Taking $\{I_j\}_j$ the partition of $[0, T]$ given by the subintervals on which $\tilde{A}(t)$ is C^2 and using the same argument as in the proof of Theorem 5, one can use Theorem 3 to show that the evolution induced by $H(t)$ satisfies

$$\|\Psi(T) - \Psi_T\| < \varepsilon.$$

5.6 Conclusions

We proposed a scheme for quantum control at the boundary and rigorously proved its controllability. It is the first time that the controllability of such a quantum system has been considered. This shows that the scheme of quantum control at the boundary is feasible. Moreover, the particular system considered presents the advantage that it could be experimentally implemented. Indeed, this quantum system represents a quantum particle moving in a spire controlled by the flux of a magnetic field that traverses the plane of the spire.

Acknowledgements J. M. P. P. is supported by QUITEMAD+, S2013/ICE-2801 and the "Juan de la Cierva - Incorporación" Proyect 2018/00002/001 and is partially supported by Spanish Ministry of Economy and Competitiveness through project DGI MTM2017-84098-P. A.B. is supported by QUITEMAD+, S2013/ICE-2801 and the UC3M University through Ph.D. program grant PIPF UC3M 01-1819 and is partially supported by Spanish Ministry of Economy and Competitiveness through project DGI MTM2017-84098-P.

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Chapter 6
Application of Lie Systems to Quantum Mechanics: Superposition Rules

José F. Cariñena, Jesús Clemente-Gallardo, Jorge A. Jover-Galtier and Javier de Lucas

Abstract We prove that t-dependent Schrödinger equations on finite-dimensional Hilbert spaces determined by t-dependent Hermitian Hamiltonian operators can be described through Lie systems admitting a Vessiot-Guldberg Lie algebra of Kähler vector fields. This result is extended to other related Schrödinger equations, e.g. projective ones, and their properties are studied through Poisson, presymplectic, and Kähler structures. This leads to deriving nonlinear superposition rules for them depending on a lower (or equal) number of solutions than standard linear ones. As an application, we study n-qubit systems and special attention is paid to the one-qubit case.

AMS Classification 34A26 (Primary) · 17B81, 34A34, 53Z05 (Secondary)

J. F. Cariñena · J. Clemente-Gallardo (✉)
Department of Theoretical Physics, Faculty of Sciences, University of Zaragoza,
c. Pedro Cerbuna 12, 50.009 Zaragoza, Spain
e-mail: jcg@unizar.es

J. F. Cariñena
IUI IUMA, University of Zaragoza, c. Pedro Cerbuna 12, 50.009 Zaragoza, Spain
e-mail: jfc@unizar.es

J. Clemente-Gallardo
IUI BIFI, University of Zaragoza, Edificio I+D, c. Mariano Esquillor s/n, 50.018 Zaragoza, Spain

J. A. Jover-Galtier
Centro Universitario de la Defensa de Zaragoza, Academia General Militar,
ctra. de Huesca s/n, 50.090 Zaragoza, Spain
e-mail: jorgejover@unizar.es

J. de Lucas
Department of Mathematical Methods in Physics, University of Warsaw,
ul. Pasteura 5, 02-093 Warszawa, Poland
e-mail: javier.de.lucas@fuw.edu.pl

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_6

6.1 Introduction

It is undoubtable that geometric techniques, e.g. Lie symmetries or jet bundles, have become a standard tool in the study of differential equations and related problems [1–4]. In particular, this work focuses on the geometric analysis of Lie systems appearing in Quantum Mechanics [4–9]. A *Lie system* is a system of first-order ordinary differential equations whose general solution can be written in terms of a generic finite family of particular solutions and a set of constants via a (generally) nonlinear function, a so-called *superposition rule* [5, 6, 8–10].

Lie systems occur in the research on the integrability of quantum systems [11], t-dependent Schrödinger equations [12], t-dependent frequency Smorodinsky-Winternitz oscillators [13], several types of Ermakov systems and Milne-Pinney equations [14–16], wave maps [17], deformation of mechanical systems [18], control systems [19], etcetera (see [20]). In geometric terms, the *Lie-Scheffers Theorem* [6, 8, 20] states that a Lie system amounts to a t-dependent vector field taking values in a finite-dimensional Lie algebra of vector fields: a *Vessiot-Guldberg Lie algebra* [20–22].

The existence of additional compatible geometric structures can be very useful. Lie systems of physical or mathematical relevance can be studied via symplectic [5, 11, 23–25], Poisson [26], k-symplectic [27], Jacobi [28], and Dirac structures [29]. This allows one to use geometric techniques to analyse their properties, e.g. their solutions [11], constants of motion [13], Lie symmetries [26], and other features [5–7, 9, 30]. Remarkably, geometric structures allow for the determination of superposition rules without solving complicated systems of partial differential equations (PDEs) or ordinary differential equations (ODEs) as standard methods [5, 9, 20]. This has also led to develop new mathematical tools so as to investigate Lie systems [27].

Although Lie systems have already been applied to quantum mechanical systems [10, 12, 31–33], there still exist many open problems. In particular, this work addresses the application of Lie systems to t-dependent Schrödinger equations governing the evolution of n-level quantum systems. This study will be carried out within the geometric formalism of Quantum Mechanics, which allows us to identify the Hilbert space $\mathcal{H}$ of an n-level quantum system with a $2n$-dimensional real Kähler manifold M_Q [34, 35]. It is important to notice that Kähler structures appear naturally as a consequence of the quantum nature of the problems under study. The pure states of the system are thus represented by points in M_Q, but this relation, however, is not one-to-one [34], as it happens in the usual Hilbert space approach. The probabilistic interpretation of the theory states that there exists an equivalence relation in $\mathcal{H} - \{0\}$, determined by the free action of the Lie groups $U(1)$ and $\mathbb{R}_+$ on $\mathcal{H}$ by multiplication. This can be easily translated to the geometric setting [35–37]. The actions of the Lie groups $U(1)$ and $\mathbb{R}_+$ on $M_{Q,0} := M_Q - \{0\}$ can be projected onto some lower-dimensional manifolds, which we collectively call *quantum quotient manifolds*. In particular, when both actions are considered together, we obtain a $2(n-1)$-dimensional Kähler manifold $\mathcal{P}$ whose elements are in a one-to-one correspondence with pure states of quantum systems.

We will analyse the geometric representation of t-dependent Schrödinger equations in these manifolds and their description as Lie systems. This enables us to obtain superposition rules without the integration of vector fields or PDEs as in standard methods [6, 9]. A crucial role is played by the use of the geometric structures in the manifolds, e.g. Kähler structures, which allows us to find superposition rules algebraically through the distributional approach devised in [6] and its refinement for Lie systems with compatible geometric structures [13]. Superposition rules for solutions of Schrödinger equation arise thus as a canonical property of the system, since they are encoded in its canonical structures. In this work, we prove that t-dependent Schrödinger equations on an n-dimensional Hilbert space $\mathcal{H}$ related to t-dependent traceless Hermitian Hamiltonian operators admit nonlinear superposition rules depending on $n-1$ particular solutions. Thus, such quantum systems can be endowed with a simple, generally nonlinear, superposition rule expressing their general solutions by means of a lower number of particular solutions than by the standard linear superposition rule associated with the Schrödinger equation on $\mathbb{C}^n$. We also prove that the projection of t-dependent Schrödinger equations onto the quotient manifolds gives rise to Lie systems admitting Vessiot-Guldberg Lie algebras of Hamiltonian vector fields relative to different geometric structures, e.g. complex, Dirac, and Poisson structures. Subsequently, the solutions of the referred to as *projective Schrödinger equations* [34, 38] are recovered. As an application of the theory, the case of 2-level quantum systems is analysed in detail. Their interest is due to its occurrence in the research on qubit models [36, 39].

6.2 Fundamentals

If not otherwise stated, we assume mathematical objects to be real, smooth, and globally defined so as to omit minor technical problems and to highlight main results. Systems of differential equations are assumed to be non-autonomous systems of ordinary differential equations.

Let $(V, [\cdot,\cdot])$ be a Lie algebra with a Lie bracket $[\cdot\,,\cdot] : V \times V \to V$. For simplicity, we will denote the Lie algebra by V if $[\cdot,\cdot]$ is known from the context. Given subsets $\mathcal{A}, \mathcal{B} \subset V$, we write $[\mathcal{A}, \mathcal{B}]$ for the linear subspace of V spanned by the Lie brackets between elements of $\mathcal{A}$ and $\mathcal{B}$, and we define $\mathrm{Lie}(\mathcal{B}, [\cdot,\cdot])$ to be the smallest Lie subalgebra of V containing $\mathcal{B}$. We will simply write $\mathrm{Lie}(\mathcal{B})$ if it is clear what we mean.

A *generalised distribution* $\mathcal{D}$ on a manifold N is an assignment to each $x \in N$ of a linear subspace $\mathcal{D}_x \subset T_xN$. We say that $\mathcal{D}$ is *regular at* $x' \in N$ if $\mathrm{r} : x \in N \mapsto \dim \mathcal{D}_x \in \mathbb{N} \cup \{0\}$ is locally constant around x'. Similarly, $\mathcal{D}$ is said to be *regular on an open* $U \subset N$ when the mapping r is constant on U. Finally, a vector field Y on N takes values in $\mathcal{D}$, in short $Y \in \mathcal{D}$, if $Y_x \in \mathcal{D}_x$ for all $x \in N$.

A *t-dependent vector field* $\mathcal{X}$ on N is a map $\mathcal{X} : (t, x) \in \mathbb{R} \times N \mapsto \mathcal{X}(t, x) \in TN$ such that $\tau_N \circ \mathcal{X} = \pi_2$, where $\pi_2 : (t, x) \in \mathbb{R} \times N \mapsto x \in N$ and τ_N is the projection of the tangent bundle onto N. For instance, if $X \in \mathfrak{X}(N)$, where $\mathfrak{X}(N)$ stands for the space of vector fields on N and $B : \mathbb{R} \to \mathbb{R}$ is a function, then $\mathcal{X}(t, x) = b(t)\, X(x)$ defines a t-dependent vector field. A t-dependent vector field $\mathcal{X}$ on N amounts to a family of vector fields $\{\mathcal{X}_t\}_{t\in\mathbb{R}}$ on N, where $\mathcal{X}_t : x \in N \mapsto \mathcal{X}(t, x) \in TN$ for all $t \in \mathbb{R}$ [20]. A t-dependent vector field $\mathcal{X} : \mathbb{R} \times N \to TN$ is *projectable* relative to a map $\pi : N \to M$ when $\mathcal{X}_t$ is projectable with respect to π for each $t \in \mathbb{R}$.

The *smallest Lie algebra* of $\mathcal{X}$ is the smallest real Lie subalgebra, $V^{\mathcal{X}}$, containing $\{\mathcal{X}_t\}_{t\in\mathbb{R}}$, namely $V^{\mathcal{X}} = \mathrm{Lie}(\{\mathcal{X}_t\}_{t\in\mathbb{R}})$. Every Lie algebra V of vector fields on N induces an integrable generalised distribution on N given by $\mathcal{D}^V := \{\mathcal{X}(x) \mid \mathcal{X} \in V, x \in N\} \subset TN$.

An *integral curve* of $\mathcal{X}$ is an integral curve $\gamma : \mathbb{R} \mapsto \mathbb{R} \times N$ of the *suspension* of $\mathcal{X}$, i.e. the vector field $\mathcal{X}(t, x) + \partial/\partial t$ on $\mathbb{R} \times N$ [40]. The curve γ always admits a reparametrisation $\bar{t} = \bar{t}(t)$ such that

$$\frac{\mathrm{d}(\pi_2 \circ \gamma)}{\mathrm{d}\bar{t}}(\bar{t}) = (\mathcal{X} \circ \gamma)(\bar{t}). \tag{6.1}$$

This system is referred to as the *associated system* of $\mathcal{X}$. Conversely, a system of first-order differential equations in normal form is always the associated system of a unique t-dependent vector field. This induces a bijection between the set of t-dependent vector fields and that of systems of first-order differential equations in normal form. This justifies denoting by $\mathcal{X}$ both a t-dependent vector field and its associated system (see [20] for details).

Definition 1 A *superposition rule* depending on m particular solutions for a system $\mathcal{X}$ on N is a function $\Phi : N^m \times N \to N$ such that the general solution, $x(t)$, of $\mathcal{X}$ can be brought into the form

$$x(t) = \Phi(x_{(1)}(t), \ldots, x_{(m)}(t); k), \tag{6.2}$$

where $x_{(1)}(t), \ldots, x_{(m)}(t)$ is a generic set of particular solutions to $\mathcal{X}$ and $k \in N$.

Example 1 It is known that a Riccati equation [9, 41], namely

$$\frac{\mathrm{d}x}{\mathrm{d}t} = a_0(t) + a_1(t)x + a_2(t)x^2, \qquad x \in \bar{\mathbb{R}} = \mathbb{R} \cup \{\infty\}, \tag{6.3}$$

where $a_0(t), a_1(t), a_2(t)$ are t-dependent real functions satisfying $a_0(t)a_2(t) \neq 0$, is such that its general solution can be brought into the form $x(t) = \Phi(x_{(1)}(t), x_{(2)}(t), x_{(3)}(t); k)$, with $\Phi : \bar{\mathbb{R}}^3 \times \bar{\mathbb{R}} \to \bar{\mathbb{R}}$ defined by

$$\Phi(u_{(1)}, u_{(2)}, u_{(3)}; k) := \frac{u_{(1)}(u_{(3)} - u_{(2)}) + k u_{(2)}(u_{(1)} - u_{(3)})}{u_{(3)} - u_{(2)} + k(u_{(1)} - u_{(3)})}, \tag{6.4}$$

where $x_{(1)}(t), x_{(2)}(t), x_{(3)}(t)$ are different particular solutions to (6.3) and $k \in \bar{\mathbb{R}}$. The solution $x_{(2)}(t)$ is obtained as the limit when $k \to \infty$.

Theorem 1 (The Lie-Scheffers Theorem [6, 8]) *A system $\mathcal{X}$ on N admits a superposition rule if and only if $\mathcal{X} = \sum_{\alpha=1}^{r} b_\alpha(t) X_\alpha$ for a family $b_1(t), \ldots, b_r(t)$ of t-dependent functions and a basis $X_1, \ldots, X_r$ of a real Lie algebra of vector fields on N.*

If $\mathcal{X}$ possesses a superposition rule, then $\mathcal{X}$ is called a *Lie system*. The associated real Lie algebra of vector fields $\langle X_1, \ldots, X_r \rangle$ is called a *Vessiot-Guldberg Lie algebra* of $\mathcal{X}$. The Lie-Scheffers Theorem amounts to saying that $\mathcal{X}$ is a Lie system if and only if $V^{\mathcal{X}}$ is finite-dimensional. This fact is the keystone of the theory of Lie systems. From a practical point of view, superposition rules make possible to solve differential equations in a simpler manner. For instance, the general solution can be obtained from a restricted set of particular solutions that can be derived straightforwardly [20] through numerical methods [9] or in other manners [20].

6.2.1 The Superposition Rule

The computation of superposition rules has been thoroughly studied in literature [6, 9, 20]. The procedure here presented is based on first integrals of diagonal prolongations of t-dependent vector fields, a fundamental notion in the geometrical description of Lie systems [6]. The geometric structures on the manifold play also an important role, as they allow us to obtain the required fist integrals [13].

Definition 2 Let $(E, N, \tau : E \to N)$ be a vector bundle. Its *diagonal prolongation* to N^m is a vector bundle $(E^{[m]}, N^m, \tau^{[m]} : E^{[m]} \to N^m)$, where $E^{[m]} := E \times \cdots \times E$ (m-times) and $\tau^{[m]}$ is the only map satisfying that $\pi_{N,j} \circ \tau^{[m]} = \tau \circ \pi_{E,j}$ for $j = 0, 1, \ldots, m-1$, with $\pi_{E,j} : E^{[m]} \to E$ and $\pi_{N,j} : N^m \to N$ being the natural projections of $E^{[m]}$ and N^m onto the j-th copy of E and N within $E^{[m]}$ and N^m, respectively.

Definition 3 Given a section $e : N \to E$ of (E, N, τ), its *diagonal prolongation* to N^m is the section $e^{[m]}$ of $(E^{[m]}, N^m, \tau^{[m]})$ obtained as the sum of the sections e of each of the copies of E within $E^{[m]}$:

$$e^{[m]} := e^{(0)} + \cdots + e^{(m-1)}. \tag{6.5}$$

Diagonal prolongations play a key role in the description of superposition rules of Lie systems. The following result gives the number of particular solutions that are needed in order to obtain the general solution of a Lie system by means of a superposition rule (see [6, 20] for details).

Theorem 2 *Let $\mathcal{X}$ be a Lie system on an n-dimensional manifold N and let V be its smallest Vessiot-Guldberg Lie algebra. The number m of particular solutions needed to obtain the general solution to $\mathcal{X}$ by means of a superposition rule is the minimum*

integer such that the diagonal prolongations of the elements in V *to* N^m *span at a generic point of* N^m *a distribution of rank* $\dim V$.

The superposition rule is obtained by means of the implicit function theorem. Let $I_1, \ldots, I_n \in C^\infty(N^{m+1})$ be n common first integrals of the diagonal prolongations of elements in V to N^{m+1} satisfying the condition

$$\det\left(\frac{\partial I_j}{\partial x_k^{(0)}}\right) \neq 0, \qquad j,k = 1,\ldots,n. \tag{6.6}$$

Then, if we assume $I_1 = k_1, \ldots, I_n = k_n$, it is possible to determine, at least in a neighbourhood of a point $x \in N^{m+1}$, the values of $x_1^{(0)}, \ldots, x_n^{(0)}$ in terms of the remaining coordinates in N^{m+1} and the values $k_1, \ldots, k_n$. This gives rise to a superposition rule for $\mathcal{X}$ of the form $\Phi(x^{(1)}, \ldots, x^{(m)};\ k_1, \ldots, k_n) = x^{(0)}$. Replacing the arguments of the superposition rule Φ by m independent particular solutions $x^1(t), \ldots, x^m(t)$ to $\mathcal{X}$, we obtain that the general solution $x(t)$ reads

$$\Phi(x^1(t), \ldots, x^m(t);\ k_1, \ldots, k_n) = x(t). \tag{6.7}$$

This procedure to obtain a superposition rule is therefore based on the first integrals of some vector fields. Here is where the additional structures that appear in particular cases of Lie systems play an important role. The properties of Lie systems can be exploited to obtain in a systematic way the first integrals that determine the superposition rule.

6.2.2 Additional Structures in Lie Systems

When $V^{\mathcal{X}}$ consists of Hamiltonian vector fields relative to some geometric structure, a so-called *compatible structure*, much more powerful methods can be devised to study Lie systems. This is the case of Lie systems with compatible symplectic, Poisson, or Dirac structures [23–25, 27, 29, 42]. This is due to the fact that the geometric structure enables us to obtain the common first-integrals used to derive the superposition rule in an algebraic manner, e.g. through Casimir elements of Lie algebras [13].

In the present work, this idea is extended to the particular case of Kähler manifolds, which have special relevance in the geometric study of Quantum Mechanics. A Kähler manifold (N, g, ω, J) is a 4-tuple where N is a differentiable manifold; g, ω, and J are tensor fields on N such that g is a Riemannian metric, ω is a symplectic form, and J is a complex structure; and the following compatibility relation is satisfied:

$$\omega(X, Y) = g(JX, Y), \tag{6.8}$$

for any pair of vector fields X, Y on N. Further information on Kähler manifold can be found in works dealing with complex manifolds [43–45]. The existence of a compatible Kähler structure makes possible to define a new type of Lie systems: the *Lie-Kähler systems*. They are defined as the Lie systems on a Kähler manifold whose Kähler structure is preserved along the evolution of the Lie system. As a consequence, the corresponding superposition rule can be derived with the help of the Kähler structure.

Definition 4 A system $\mathcal{X}$ on a Kähler manifold (N, ω, g, J) is called a *Lie-Kähler system* if $\mathcal{X}$ admits a Lie-Hamilton structure with respect to the Poisson bivector determined by the symplectic form ω and preserves the complex structure, i.e. $\mathcal{L}_{\mathcal{X}_t} J = 0$ for any $t \in \mathbb{R}$.

From the definition, it is simple to prove:

Proposition 1 *Consider a Kähler manifold* (N, ω, g, J). *If* $\mathcal{X}$ *is a Lie-Kähler system, then, for any* $t \in \mathbb{R}$, *each vector field* $\mathcal{X}_t$ *is a Killing vector field with respect to the metric tensor* g.

Proof Tensor fields ω, g, and J are related by (6.8). If the Lie derivatives of ω and J relative to a vector field of the Vessiot-Guldberg Lie algebra $\mathcal{X}$ is zero, then the Lie derivative of g relative to the same vector field is also zero. The proposition follows as a consequence.

The following result could be restated as an alternate definition of Lie-Kähler systems.

Proposition 2 *Consider a Kähler manifold* (N, ω, g, J). *If* $\mathcal{X}$ *is a Lie-Kähler system, then any vector field of one of the smallest Lie algebra of* $\mathcal{X}$ *is an infinitesimal symmetry of the Kähler structure on* N.

Proof This result is a consequence of the definition of Lie-Kähler systems and Proposition 1.

6.3 The Geometrical Description of Quantum Mechanics

From a physical point of view, a very relevant example of Lie-Kähler systems corresponds to finite-dimensional quantum dynamical systems. For them, Kähler structures encode in geometrical terms the Hermitian structure of the Hilbert space, while t-dependent Schrödinger equation defines the corresponding Lie system. We briefly present now the geometrical formulation of quantum mechanics which has been developed during the last forty years (see [35–37, 43] for a deeper analysis of the formalism) in order to make these relations explicit.

6.3.1 The Linear, Complex, and Hermitian Structure

The geometric formalism of quantum mechanics is based on the identification of the Hilbert space $\mathcal{H}$, with Hermitian product $\langle \cdot, \cdot \rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$, associated with an n-level quantum system with a real $2n$-dimensional differentiable manifold M_Q [46]. Thus, every vector $|\psi\rangle \in \mathcal{H}$ is identified with a point $\psi \in M_Q$. Any basis $\{|e_j\rangle\}$ in $\mathcal{H}$ defines a real global chart (q_j, p_j) on M_Q as follows

$$\langle e_j, \psi \rangle = \frac{1}{\sqrt{2}} \left(q_j(\psi) + \mathrm{i}\, p_j(\psi) \right), \qquad j = 1, \ldots, n, \quad \forall \psi \in M_Q, \tag{6.9}$$

As $\mathcal{H} \simeq \mathbb{R}^{2n}$ as $\mathbb{R}$-linear spaces, there exists at each $\psi \in M_Q$ an $\mathbb{R}$-linear isomorphism between $\mathcal{H}$ and the tangent vector space $T_\psi M_Q$ at each $\psi \in M_Q$. Thus, operations on $\mathcal{H}$ can be encoded in terms of tensor fields. For instance, multiplication by the imaginary unit i can be represented by a linear operation on the elements of $T_\psi M_Q$ which defines a complex structure J_ψ and hence a (1,1)-tensor field on M_Q. In a similar way, the Hermitian product on $\mathcal{H}$ allows us to define two tensor fields g, ω on M_Q, as its real and imaginary parts:

$$\begin{aligned} &g_\psi(\phi_\psi, \phi'_\psi) := 2\mathrm{Re}\, \langle \phi, \phi' \rangle \qquad \omega_\psi(\phi_\psi, \phi'_\psi) := 2\mathrm{Im}\, \langle \phi, \phi' \rangle, \\ &\forall \psi \in M_Q, \ \forall \phi, \phi' \in T_\psi M_Q. \end{aligned} \tag{6.10}$$

In the coordinate system (6.9), these tensor fields read

$$\begin{aligned} g &= \sum_{j=1}^{n} \left(\mathrm{d}q_j \otimes \mathrm{d}q_j + \mathrm{d}p_j \otimes \mathrm{d}p_j \right), \quad \omega = \sum_{j=1}^{n} \mathrm{d}q_j \wedge \mathrm{d}p_j, \\ J &= \sum_{j=1}^{n} \left(\mathrm{d}q_j \otimes \frac{\partial}{\partial p_j} - \mathrm{d}p_j \otimes \frac{\partial}{\partial q_j} \right), \end{aligned} \tag{6.11}$$

with $u \wedge v = u \otimes v - v \otimes u$. The tensor field g becomes a Euclidean metric on $\mathbb{R}^{2n}$, and it defines a norm $\| \cdot \|$ on M_Q, which is related to the norm on $\mathcal{H}$ defined by its natural Hermitian product. On the other hand, the tensor field ω becomes a symplectic structure on $\mathbb{R}^{2n}$ with Darboux coordinates (q_j, p_j). The three tensor fields satisfy the following relations

$$\begin{aligned} &g(JX, JY) = g(X, Y), \ \omega(JX, JY) = \omega(X, Y), \ \omega(X, Y) = g(JX, Y), \\ &\forall X, Y \in \mathfrak{X}(M_Q). \end{aligned}$$

Thus, the Hermitian product on $\mathcal{H}$ leads to a Kähler structure on M_Q, which is typical of quantum models and richer than the standard symplectic one appearing in classical mechanics.

Both g and ω are non-singular tensor fields, thus they define bundle isomorphisms between TM_Q and T^*M_Q. As a consequence, it is possible to find two 2-contravariant tensor fields G and Ω that are the inverses of g and ω. Their expressions in local coordinates are

$$G = \sum_{j=1}^{n} \left(\frac{\partial}{\partial q_j} \otimes \frac{\partial}{\partial q_j} + \frac{\partial}{\partial p_j} \otimes \frac{\partial}{\partial p_j} \right), \qquad \Omega = \sum_{j=1}^{n} \frac{\partial}{\partial q_j} \wedge \frac{\partial}{\partial p_j}. \tag{6.12}$$

These tensor fields define a Poisson bracket and a commutative bracket on $C^\infty(M_Q)$, respectively:

$$\{f, g\} := \Omega(\mathrm{d}f, \mathrm{d}g), \qquad \{f, g\}_+ := G(\mathrm{d}f, \mathrm{d}g), \qquad \forall f, g \in C^\infty(M_Q). \tag{6.13}$$

A third element in the description of the Hilbert space structure of $\mathcal{H}$ is its $\mathbb{R}$-linear structure. Geometrically, it is induced by the so-called *dilation vector field* defined by $\Delta : \psi \in M_Q \mapsto (\psi, \psi) \in TM_Q$, where we use that, as M_Q is a linear space, $TM_Q \simeq M_Q \times M_Q$. Moreover, the *phase-change vector field* takes the form $\Gamma : \psi \in M_Q \mapsto (\psi, J_\psi \psi) \in T_\psi M_Q$. These vector fields satisfy the relation $\Gamma = J\Delta$. Their expressions in the coordinates (q_j, p_j) are

$$\Delta = \sum_{j=1}^{n} \left(q_j \frac{\partial}{\partial q_j} + p_j \frac{\partial}{\partial p_j} \right), \qquad \Gamma = \sum_{j=1}^{n} \left(q_j \frac{\partial}{\partial p_j} - p_j \frac{\partial}{\partial q_j} \right). \tag{6.14}$$

6.3.2 Observables: Hamiltonian Dynamics and Killing Vector Fields

The real vector space $\mathrm{Herm}(\mathcal{H})$ of physical observables on $\mathcal{H}$, i.e. Hermitian operators on $\mathcal{H}$, can also be given a tensor description. Every observable $A \in \mathrm{Herm}(\mathcal{H})$ gives rise to a real function on M_Q of the form

$$f_A(\psi) := \langle \psi, A\psi \rangle, \qquad \psi \in M_Q. \tag{6.15}$$

It is immediate to verify that the two algebraic operations in $\mathrm{Herm}(\mathcal{H})$ given by

$$[\![A, B]\!] := -\mathrm{i}\,(AB - BA), \qquad [A, B]_+ := AB + BA, \tag{6.16}$$

are related to the brackets of functions on M_Q as follows

$$\{f_A, f_B\} = \Omega(\mathrm{d}f_A, \mathrm{d}f_B) = f_{[\![A,B]\!]}, \qquad \{f_A, f_B\}_+ = G(\mathrm{d}f_A, \mathrm{d}f_B) = f_{[A,B]_+}.$$

As in any Poisson manifold, each Hamiltonian vector field, let us say X_f, can be associated with a function $f \in C^\infty(M_Q)$ as follows:

$$X_f := -\Omega(\mathrm{d}f, \cdot) = \{\cdot, f\}. \tag{6.17}$$

In the particular case of functions in the form of (6.15), their Hamiltonian vector fields satisfy the following commutation rule

$$[X_{f_A}, X_{f_B}] = -X_{f_{[\![A,B]\!]}}. \tag{6.18}$$

Consider the particular case of the Hamiltonian vector field X_{f_H} associated with the quadratic form $f_H(\psi) := \langle \psi, H\psi \rangle$, where H is the Hamiltonian operator of a physical system. Its integral curves correspond to the solutions of the Schrödinger equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle, \tag{6.19}$$

where we assumed, as hereafter, $\hbar = 1$. The evolution operator $t \mapsto U_t$ defines an isometry of the Hermitian product on $\mathcal{H}$. Hence, each U_t leaves invariant its real and imaginary parts. Since each U_t is $\mathbb{C}$-linear, its induced action onto M_Q also leaves invariant ω, J, and g. Therefore, X_{f_H} is also a Killing vector field relative to g giving rise to a Kähler vector field.

6.3.3 Projective Hilbert Spaces as Kähler Manifolds

The probabilistic interpretation of Quantum Mechanics requires to deal with an equivalence relation in the Hilbert space of the system, namely

$$|\psi_1\rangle, |\psi_2\rangle \in \mathcal{H}_0 := \mathcal{H}\backslash\{0\}, \quad |\psi_1\rangle \sim |\psi_2\rangle \Leftrightarrow |\psi_2\rangle = \lambda|\psi_1\rangle, \quad \lambda \in \mathbb{C}_0 := \mathbb{C}\backslash\{0\}. \tag{6.20}$$

Therefore, elements describing pure quantum states must be rays rather than vectors. In particular, for finite-dimensional systems, the space of pure states is not $\mathbb{C}^n$ but the projective space $\mathbb{CP}^{n-1}$.

The equivalence relation (6.20) coincides with the one defined by the action of the group $(\mathbb{C}_0, \cdot)$ on $M_{Q,0} := M_Q - \{0\}$, with 0 being the point in M_Q representing the zero vector in $\mathcal{H}$, the orbits of the action being the equivalence classes. The group is Abelian and isomorphic to the direct product group of $(\mathbb{R}_+, \cdot)$ by the unitary group $U(1)$. The fundamental vector fields of this action are spanned by the dilation Δ and phase-change Γ vector fields. They give rise to a regular foliation $\mathcal{F}_{\Delta,\Gamma}$ on $M_{Q,0}$. Observe that, as $M_{Q,0}$ is an open submanifold of M_Q, any geometric object on M_Q can be restricted to $M_{Q,0}$. From now onwards, this restriction is implicitly assumed, thus simplifying the notation.

The foliation $\mathcal{F}_{\Delta,\Gamma}$ defines a projection $\pi : M_{Q,0} \to \mathcal{P}$ onto its set of leaves $\mathcal{P}$. The points of $\mathcal{P}$ represent, geometrically, the points of the projective space and therefore they are identified with pure states of the quantum system. The notation from equivalence relations can be kept, thus we will denote elements in $\mathcal{P}$ by $[\psi] := \pi(\psi)$. Due to the commutativity of Δ and Γ, their respective flows commute. Thus, it is possible to carry out the projection $\pi : M_{Q,0} \to \mathcal{P}$ in two steps and in any order.

If $\mathcal{F}_\Gamma$ and $\mathcal{F}_\Delta$ denote respectively the regular foliations of $M_{Q,0}$ by Γ and Δ, then the set of leaves of $\mathcal{F}_\Gamma$ will be denoted by $\mathcal{R}$, being $\pi_{M\mathcal{R}} : M_{Q,0} \to \mathcal{R}$ the corresponding projection. Similarly, $\mathcal{Q}$ will stand for the set of leaves of $\mathcal{F}_\Delta$, being $\pi_{M\mathcal{Q}} : M_{Q,0} \to \mathcal{Q}$ the corresponding projection. For every $\psi \in M_{Q,0}$, its images by $\pi_\mathcal{R}$ and $\pi_\mathcal{Q}$ will be denoted by $[\psi]_\mathcal{R} \in \mathcal{R}$ and $[\psi]_\mathcal{Q} \in \mathcal{Q}$, respectively.

Proposition 3 *The manifold $\mathcal{Q}$ is diffeomorphic to the unit sphere $S^{2n-1} \subset \mathbb{R}^{2n}$, where n denotes the complex dimension of the initial Hilbert space.*

Proof The manifold $M_{Q,0}$ is a $2n$-dimensional manifold with a global chart $\phi_E : M_{Q,0} \to \mathbb{R}^{2n}\backslash\{0\}$, defined as in (6.9). Elements of $\mathcal{Q}$ are the orbits of Δ. It is possible to consider the immersion $\imath_\mathcal{Q} : \mathcal{Q} \to M_Q$ that associates each orbit of the flow of Δ with the only point within it having a unit norm. As the norm in M_Q is equivalent to the canonical norm in $\mathbb{R}^{2n}$, the set $\imath_\mathcal{Q}(\mathcal{Q})$ is mapped onto the points of $\mathbb{R}^{2n}$ with unit norm and hence $(\phi_E \circ \imath_\mathcal{Q})(\mathcal{Q}) \simeq S^{2n-1}$.

Both $\mathcal{R}$ and $\mathcal{Q}$ are $(2n-1)$-dimensional differentiable manifolds. New projections can be established on each manifold, thus completing the projection onto the manifold $\mathcal{P}$, previously defined.

Proposition 4 *The vector field Δ projects onto $\mathcal{R}$, defining a regular foliation. Likewise, the vector field Γ projects onto $\mathcal{Q}$, defining also a regular foliation. The diagram shown in Fig. 6.1 is commutative, i.e. the projections $\pi_{\mathcal{R}\mathcal{P}} : \mathcal{R} \to \mathcal{P}$ and $\pi_{\mathcal{Q}\mathcal{P}} : \mathcal{Q} \to \mathcal{P}$ satisfy that*

$$\pi_{\mathcal{R}\mathcal{P}} \circ \pi_{M\mathcal{R}} = \pi_{\mathcal{Q}\mathcal{P}} \circ \pi_{M\mathcal{Q}} = \pi. \tag{6.21}$$

Proof The commutativity of both vector fields makes possible to project Δ onto $\mathcal{R}$, and also Γ onto $\mathcal{Q}$. As Δ and Γ are non-zero at every point of $M_{Q,0}$, their respective projections to $\mathcal{R}$ and $\mathcal{Q}$ define regular foliations. The commutativity of the diagram is a straightforward consequence.

An additional immersion can be defined. Namely, the projective manifold $\mathcal{P}$ can be naturally mapped into the manifold $\mathcal{R}$, as it is shown next.

Proposition 5 *There exists a embedding $\imath_\mathcal{P} : \mathcal{P} \to \mathcal{R}$ such that $\pi_{\mathcal{R}\mathcal{P}} \circ \imath_\mathcal{P} = \mathrm{Id}_\mathcal{P}$.*

Proof Due to the commutativity of the diagram in Fig. 6.1, for every element of $\mathcal{P}$ there exists an element of $\mathcal{Q}$ projecting to it under $\pi_{\mathcal{Q}\mathcal{P}}$. Let $f_{\mathcal{Q}\mathcal{R}} : \mathcal{Q} \to \mathcal{R}$ be the map $f_{\mathcal{Q}\mathcal{R}} := \pi_{M\mathcal{R}} \circ \imath_\mathcal{Q}$. Hence, $\pi_{\mathcal{R}\mathcal{P}} \circ f_{\mathcal{Q}\mathcal{R}}(\mathcal{Q}) = \mathcal{P}$ and $\pi_{\mathcal{R}\mathcal{P}}|_{f_{\mathcal{Q}\mathcal{R}}(\mathcal{Q})} : f_{\mathcal{Q}\mathcal{R}}(\mathcal{Q}) \to \mathcal{P}$ is surjective. It can be shown that it is also injective. Take $\psi_1, \psi_2 \in$

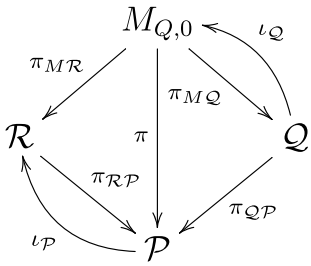

Fig. 6.1 The diagram illustrates the manifolds appearing in the study of quantum systems. The projections and natural immersions are indicated

$\iota_{\mathcal{Q}}(\mathcal{Q})$, which implies that $\|\psi_1\| = \|\psi_2\|$. Consider their equivalence classes $[\psi_1]_{\mathcal{R}}$, $[\psi_2]_{\mathcal{R}} \in \mathcal{R}$. Then, if $\pi_{\mathcal{R}\mathcal{P}}([\psi_1]_{\mathcal{R}}) = \pi_{\mathcal{R}\mathcal{P}}([\psi_2]_{\mathcal{R}})$, necessarily $|\psi_1\rangle = e^{\mathrm{i}\alpha}|\psi_2\rangle$ with $\alpha \in \mathbb{R}$. As equivalence classes in $\mathcal{R}$ are defined by the action of the $U(1)$, it is immediate that $[\psi_1]_{\mathcal{R}} = [\psi_2]_{\mathcal{R}}$. Therefore, $\pi_{\mathcal{R}\mathcal{P}}$ is a bijection when restricted to $f_{\mathcal{Q}\mathcal{R}}(\mathcal{Q})$. The inverse map, defined as $\iota_{\mathcal{P}}$, is thus a differentiable embedding.

The tensor fields G and Ω on $M_{Q,0}$ induced by (6.12) cannot be projected onto $\mathcal{P}$ since they are not invariant under Δ. We thus define two new tensor fields by

$$G_{\mathcal{P}} := f_I(\psi)G - \frac{(\Delta \otimes \Delta + \Gamma \otimes \Gamma)}{2}, \quad \Omega_{\mathcal{P}} := f_I(\psi)\Omega - \frac{(\Delta \otimes \Gamma - \Gamma \otimes \Delta)}{2}. \tag{6.22}$$

which are projectable and also preserve the algebraic structures of functions [36, 37]. The projected tensor fields correspond to the Fubiny-Study metric of the complex projective space [47, 48] and the symplectic and complex structure tensors giving rise to the canonical Kähler structure on $\mathcal{R}$. Regarding observables, quadratic functions f_A defined in (6.15) are not invariant by Δ and Γ. Instead, observables are to be represented by expectation value functions, defined on $M_{Q,0}$ as

$$e_A(\psi) := \frac{\langle \psi, A\psi \rangle}{\langle \psi, \psi \rangle}. \tag{6.23}$$

These functions are projectable, i.e. they correspond to pull-backs of functions on $\mathcal{P}$.

6.4 Lie-Kähler Systems in Quantum Mechanics

It is known that Lie systems appear in the geometric study of t-dependent Schrödinger equations [12, 31–33]. The expression of this equation in natural units (with $\hbar = 1$) is

$$\mathrm{i}\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle, \quad t \in \mathbb{R}, \tag{6.24}$$

where $H(t)$ is a Hermitian operator on $\mathcal{H}$ for every t, which stands for the physical time parameter. This operator is called the *t-dependent Hamiltonian of the system*. The aim of this section is to prove that, for finite-dimensional systems, it is possible to describe such an equation in terms of a Lie system.

Definition 5 A t-dependent Hamiltonian $H(t)$ is called a *quantum Lie system* if there exists a set of r real t-dependent functions $b_1(t), \ldots, b_r(t)$ such that

$$H(t) = \sum_{j=1}^{r} b_j(t) H_j, \tag{6.25}$$

where the Hermitian operators $H_1, \ldots, H_r$ span a real finite-dimensional Lie algebra V^H, called a *quantum Vessiot-Guldberg Lie algebra* of $H(t)$.

Proposition 6 *Any t-dependent Hamiltonian on a finite-dimensional Hilbert space is a quantum Lie system.*

Proof If the Hilbert space $\mathcal{H}$ is finite-dimensional, any basis $\{H_1, \ldots, H_n\}$ for $\mathrm{Herm}(\mathcal{H})$ makes possible to write a generic t-dependent Hamiltonian $H(t)$ in the form (6.25). For particular cases, it may be possible to find smaller quantum Vessiot-Guldberg Lie algebras for $H(t)$.

It is to be remarked that sometimes the Vessiot–Lie algebra of the t-dependent Hamiltonian may be lower-dimensional and this simplifies computations. This is the case we study next.

Theorem 3 *Consider a quantum Lie system $H(t)$ on a finite-dimensional Hilbert space $\mathcal{H}$, with $V^H = \mathrm{Lie}(H_1, \ldots, H_r)$ being a quantum Vessiot-Guldberg Lie algebra. The t-dependent vector field $\mathcal{X}^H$ on the manifold M_Q defined by*

$$\mathcal{X}^H_t = \sum_{j=1}^{r} b_j(t) X_j, \qquad \text{with } X_j := X_{f_{H_j}}, \quad j = 1, \ldots, r, \tag{6.26}$$

is a Lie-Kähler system on M_Q. The associated system of $\mathcal{X}^H$ is its t-dependent Schrödinger equation.

Proof Hamiltonian vector fields satisfy the commutation relation (6.18). If the Lie bracket of V^H is $[\![H_j, H_k]\!] = \sum_l c_{jkl} H_l$, then

$$[X_j, X_k] = -X_{f_{[\![H_j, H_k]\!]}} = -\sum_{l=1}^{r} c_{jkl} X_l, \quad j, k = 1, 2, \ldots, r.$$

Therefore, $\mathrm{Lie}(X_1, \ldots, X_r)$ is a finite-dimensional Lie algebra isomorphic to V^H. As a consequence of the Lie-Scheffers Theorem, $\mathcal{X}^H$ is a Lie system with $\mathrm{Lie}(X_1, \ldots, X_r)$ as a Vessiot-Guldberg Lie algebra.

For each $t \in \mathbb{R}$, the vector field $\mathcal{X}_t^H$ is Hamiltonian with respect to ω and Hamiltonian function on M_Q associated with the operator $\sum_{j=1}^r b_j(t)H_j = H(t)$. As a consequence, its associated differential equation is (6.24), thus proving the relation between Lie systems and the t-dependent Schrödinger equation.

6.4.1 2-Level Lie Systems

The Hilbert space of a 2-level system is isomorphic to $\mathbb{C}^2$ with its natural Hermitian structure. Observables are represented by matrices in Herm(2), for which a basis $\{\sigma_0, \sigma_1, \sigma_2, \sigma_3\}$ is defined by

$$\sigma_0 = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \ \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{6.27}$$

A quantum Lie system $H(t)$ thus takes the form

$$H(t) = B_0(t)\sigma_0 + \sum_{j=1}^{3} B_j(t)\sigma_j. \tag{6.28}$$

Physically, this Hamiltonian models a $\frac{1}{2}$-spin system coupled with a t-dependent magnetic field given by $(B_1(t), B_2(t), B_3(t))$ and a drag term due to $B_0(t)$. The t-dependent Hamiltonian $H(t)$ is therefore a quantum Lie system. It determines a t-dependent Schrödinger equation of the form (6.24) in $\mathbb{C}^2$ [6, 49].

Consider now the geometric formalism presented in Sect. 6.3. The Hilbert space $\mathcal{H} \cong \mathbb{C}^2$ is identified with a 4-dimensional differentiable manifold M_Q, where a global chart with coordinates (q_1, p_1, q_2, p_2) exists, defined as in (6.9). The quantum Lie system $H(t)$ defines a Lie-Kähler system $\mathcal{X}^H$ on M_Q:

$$\mathcal{X}^H = \sum_{j=0}^{3} B_j(t)X_j, \tag{6.29}$$

The associated system of $\mathcal{X}^H$ is the geometrical equivalent of the Schrödinger equation (6.24) for the 2-level quantum system. The vector fields X_0, X_1, X_2, X_3 span the Vessiot-Guldberg Lie algebra of $\mathcal{X}^H$. The commutation relations can be directly computed by their coordinate expressions:

$$
\begin{aligned}
X_0 &= p_1\frac{\partial}{\partial q_1} - q_1\frac{\partial}{\partial p_1} + p_2\frac{\partial}{\partial q_2} - q_2\frac{\partial}{\partial p_2},\\
X_1 &= p_2\frac{\partial}{\partial q_1} - q_2\frac{\partial}{\partial p_1} + p_1\frac{\partial}{\partial q_2} - q_1\frac{\partial}{\partial p_2},\\
X_2 &= -q_2\frac{\partial}{\partial q_1} - p_2\frac{\partial}{\partial p_1} + q_1\frac{\partial}{\partial q_2} + p_1\frac{\partial}{\partial p_2},\\
X_3 &= p_1\frac{\partial}{\partial q_1} - q_1\frac{\partial}{\partial p_1} - p_2\frac{\partial}{\partial q_2} + q_2\frac{\partial}{\partial p_2}.
\end{aligned}
\tag{6.30}
$$

As expected, these vector fields span a 4-dimensional Lie algebra isomorphic to Herm(2):

$$
[X_0, \cdot] = 0, \quad [X_1, X_2] = -2X_3, \quad [X_2, X_3] = -2X_1, \quad [X_3, X_1] = -2X_2. \tag{6.31}
$$

The vector fields X_0, X_1, X_2, X_3 are Hamiltonian with respect to ω. Their Hamiltonian functions are

$$
\begin{aligned}
h_0(\psi) &= \langle \psi, \sigma_0 \psi \rangle = \frac{1}{2}(q_1^2 + p_1^2 + q_2^2 + p_2^2),\\
h_1(\psi) &= \langle \psi, \sigma_1 \psi \rangle = q_1 q_2 + p_1 p_2,\\
h_2(\psi) &= \langle \psi, \sigma_2 \psi \rangle = q_1 p_2 - p_1 q_2,\\
h_3(\psi) &= \langle \psi, \sigma_3 \psi \rangle = \frac{1}{2}(q_1^2 + p_1^2 - q_2^2 - p_2^2),
\end{aligned}
\tag{6.32}
$$

with $\iota_{X_\alpha}\omega := \omega(X_\alpha, \cdot) = \mathrm{d}h_\alpha$ for $\alpha = 0, 1, 2, 3$. Notice that h_1, h_2, h_3 are functionally independent, but $h_0^2 = h_1^2 + h_2^2 + h_3^2$. The Hamiltonian functions span a Lie algebra isomorphic to Herm(2):

$$
\{h_0, \cdot\} = 0, \qquad \{h_1, h_2\} = 2h_3, \qquad \{h_2, h_3\} = 2h_1, \qquad \{h_3, h_1\} = 2h_2. \tag{6.33}
$$

The vector fields X_0, X_1, X_2, and X_3 are Killing vector fields with respect to g, namely $\mathcal{L}_{X_\alpha} g = 0$ for $\alpha = 0, 1, 2, 3$. Using this, we can prove in an intrinsic geometric way that

$$
\begin{aligned}
&I_1 = g(X_0, X_0), \quad I_2 = g(X_1, X_1) + g(X_2, X_2) + g(X_3, X_3),\\
&I_3 = h_1^2 + h_2^2 + h_3^2, \quad I_4 = h_0
\end{aligned}
\tag{6.34}
$$

are constants of the motion for $\mathcal{X}^H$. This example is relevant because it illustrates how to define the above constants of the motion geometrically in terms of g and the Hamiltonian functions due to ω.

6.4.2 Schrödinger Equations and Lie-Kähler Systems

Theorem 4 *Every t-dependent Schrödinger equation on a finite-dimensional Hilbert space $\mathcal{H}$ defines a Lie-Kähler system on the associated Kähler manifold M_Q with a Vessiot-Guldberg Lie algebra that is isomorphic to a subalgebra of* $\mathrm{Herm}(\mathcal{H})$.

Proof The relation between t-dependent Schrödinger equations on $\mathcal{H}$ and Lie systems on M_Q was clarified in Theorem 3. The Vessiot-Guldberg Lie algebra of $\mathcal{X}^H$ is isomorphic to the quantum Vessiot-Guldberg Lie algebra V^H of $H(t)$, which in turn is a subalgebra of $\mathrm{Herm}(\mathcal{H})$, as proved in Proposition 6. The preservation of the Kähler structure of M_Q remains from the results given in Sect. 6.3.2. From this follows that the Vessiot-Guldberg Lie algebra of $\mathcal{X}^H$ consists of Hamiltonian vector fields and Killing vector fields relative to the Kähler structure on M_Q. Then, $\mathcal{X}^H$ is a Lie-Kähler system.

Proposition 7 *The space $I^{\mathcal{X}}$ of time-independent constants of motion for a Lie-Kähler system $\mathcal{X}$ is a Poisson algebra with respect to the Poisson bracket of the Kähler structure and a commutative algebra relative to the bracket induced by the Riemannian structure.*

Proof This proposition stems from a simple differential geometric computation. Lie derivatives and contractions satisfy the following relation [50, 51]:

$$[\mathcal{L}_X, \iota_Y] = \iota_{[X,Y]}, \tag{6.35}$$

for any pair of vector fields X, Y.

Any time-independent constant of motion $f \in I^{\mathcal{X}}$ satisfies $\mathcal{X}_t(f) = \mathcal{L}_{\mathcal{X}_t}(f) = 0$ for any $t \in \mathbb{R}$. On the other hand, the Hamiltonian vector field X_f associated with f satisfies $\mathrm{d}f = \iota_{X_f}\omega$, with ω the symplectic structure on the Kähler manifold. The two relations combined yield the following result:

$$\mathrm{d}(\mathcal{L}_{\mathcal{X}_t}(f)) = \mathcal{L}_{\mathcal{X}_t}(\mathrm{d}f) = 0 \Rightarrow \mathcal{L}_{\mathcal{X}_t}(\iota_{X_f}\omega) = 0 \Rightarrow \iota_{[\mathcal{X}_t, X_f]}\omega = 0,$$

where the fact that $\mathcal{X}$ is a Lie-Kähler system, hence $\mathcal{L}_{\mathcal{X}_t}\omega = 0$, has been used.

The Poisson bracket of any two functions f, f', as defined in (6.13), is given by

$$\{f, f'\} = \omega(X_f, X_{f'}). \tag{6.36}$$

Its Lie derivative with respect to a vector field $Y \in \mathfrak{X}(M_Q)$ satisfies the following relation [40, p.117]:

$$\begin{aligned}\mathcal{L}_Y(\{f, f'\}) = \mathcal{L}_Y(\omega(X_f, X_{f'}) &= (\mathcal{L}_Y\omega)(X_f, X_{f'}) \\ &+ \omega([Y, X_f], X_{f'}) + \omega(X_f, [Y, X_{f'}]).\end{aligned}$$

In particular, this relation holds for $Y = \mathcal{X}_t$. If f and f' are constants of motion and as Y is a Hamiltonian vector field, $[Y, X_f]$ is the Hamiltonian vector field of the function

$Yf = 0$ and the right-hand side of the equality is zero, hence

$$\mathcal{L}_{\mathcal{X}_t}(\{f, f'\}) = 0, \quad \forall f, f' \in I^{\mathcal{X}}. \tag{6.37}$$

Therefore $\{f, f'\}$ is also a constant of motion. Likewise, the symmetric product defined by the metric g provided by the Kähler structure satisfies a similar relation.

6.5 Lie Systems on the Quantum Quotient Manifolds

As fully explained in Sect. 6.3.3, the proper description of the states of quantum systems requires an analysis of the fibration $\mathcal{F}_{\Delta,\Gamma}$ of M_Q obtained by integrating the distribution spanned by the vector fields Γ and Δ. This fibration is regular on $M_{Q,0} = M_Q - \{0\}$, and we can define a projection onto the manifold of leaves of the foliation. Furthermore, as Δ, Γ commute, the projection can be decomposed into two steps, and carried out in any order.

As a result, different quotient manifolds $\mathcal{R}$, $\mathcal{Q}$, and $\mathcal{P}$ are obtained. They are collectively referred to as the quantum quotient manifolds. The diagram in Fig. 6.2 reproduces the existing maps and immersions. Also, the relevant structures in each manifold are indicated. The following sections consider the properties of Lie systems determined by t-dependent Schrödinger equations on each of the quantum quotient manifolds.

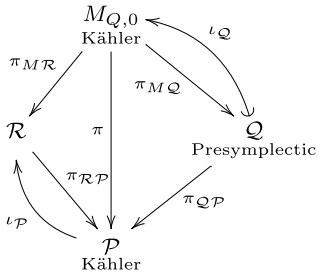

Fig. 6.2 The diagram illustrates the manifolds appearing in the study of quantum systems. The projections and natural immersions are indicated. Each manifold is labelled according to the relevant geometric structure it possesses. These structures are useful in the determination of superposition rules for Lie systems

6.5.1 Lie Systems on the Manifold $\mathcal{Q}$

Consider the immersion $\iota_{\mathcal{Q}} : \mathcal{Q} \to M_{Q,0}$, as indicated in Fig. 6.2. Since the unitary evolution in $\mathcal{H}$ determined by the Schrödinger equation preserves the norm of vectors, its geometrical counterpart on $M_{Q,0}$ leaves the unity sphere $\iota_{\mathcal{Q}}(\mathcal{Q})$ invariant. Thus, it seems natural at first to restrict the associate Lie-Kähler system with the unity sphere $\mathcal{Q}$. Nevertheless, as shown below, such a restriction is generally no longer neither a Lie-Kähler system nor a Lie-Hamilton one.

Proposition 8 *Consider the Lie-Kähler system $\mathcal{X}^H$ on $M_{Q,0}$ determined by a quantum Lie system $H(t)$. The Lie-Kähler system $\mathcal{X}^H$ can be projected onto $\mathcal{Q}$ giving rise to a Lie system $\mathcal{X}^H_{\mathcal{Q}}$ possessing a Vessiot-Guldberg Lie algebra $V_{\mathcal{Q}}$ of Hamiltonian vector fields with respect to the presymplectic form $\omega_{\mathcal{Q}} := \iota^*_{\mathcal{Q}}\omega$ with $\iota_{\mathcal{Q}} : \mathcal{Q} \hookrightarrow M_Q$. If $V^{\mathcal{X}^H_{\mathcal{Q}}} = V_{\mathcal{Q}}$, then $\mathcal{X}^H_{\mathcal{Q}}$ is not a Lie-Hamilton system.*

Proof For a generic quantum Lie system $H(t)$, the Vessiot-Guldberg Lie algebra V of $\mathcal{X}^H$ is the Lie algebra of fundamental vector fields of the unitary action on M_Q, namely $\varphi_M : U(\mathcal{H}) \times M_Q \to M_Q$, as proved in Proposition 6. Recall that unitary action preserves the Hermitian product in $\mathcal{H}$. Hence, the norm $\|\psi\|$ induced by the metric of $\mathcal{H}$ is invariant under φ_M and, in consequence, a first-integral of its fundamental vector fields, which span $V^{\mathcal{X}^H}$. The restrictions of the elements of $V^{\mathcal{X}^H}$ to $\mathcal{Q}$ become tangent to $\iota_{\mathcal{Q}}(\mathcal{Q})$ and therefore they span a finite-dimensional Lie algebra of vector fields $V_{\mathcal{Q}}$ on $\mathcal{Q}$. The Lie-Kähler system $\mathcal{X}^H$, being generated by the elements in $V^{\mathcal{X}^H}$, can also be restricted to $\iota_{\mathcal{Q}}(\mathcal{Q})$. It gives rise to a Lie system $\mathcal{X}^H_{\mathcal{Q}}$ on $\mathcal{Q}$ admitting a Vessiot-Guldberg Lie algebra $V_{\mathcal{Q}}$.

The embedding $\iota_{\mathcal{Q}} : \mathcal{Q} \to M_Q$ induces a presymplectic structure $\omega_{\mathcal{Q}} = \iota^*_{\mathcal{Q}}\omega$ on $\mathcal{Q}$, where ω is the natural symplectic structure on M_Q. Since the elements of $V^{\mathcal{X}^H}$ are Hamiltonian vector fields on M_Q with Hamiltonian functions $h_H(\psi) = \langle \psi, H\psi \rangle$ with $H \in \mathrm{Herm}(\mathcal{H})$, their restrictions to $\mathcal{Q}$ are Hamiltonian relative to the presymplectic form $\omega_{\mathcal{Q}}$ with Hamiltonian functions $\iota^*_{\mathcal{Q}} h_H$. Therefore, the algebra $V_{\mathcal{Q}}$ on $\mathcal{Q}$ is composed of Hamiltonian vector fields relative to the presymplectic structure $\omega_{\mathcal{Q}}$.

As $\mathcal{Q}$ is an orbit of φ_M, then $T\mathcal{Q} = D^{V^{\mathcal{X}^H}}|_{\mathcal{Q}}$, which is a distribution with odd rank $2n-1$. From assumption, $V^{X_{\mathcal{Q}}} = V_{\mathcal{Q}}$, and hence $D^{X_{\mathcal{Q}}} = D^{V_{\mathcal{Q}}} = D^{V^{\mathcal{X}^H}}|_{\mathcal{Q}} = T\mathcal{Q}$. The so-called no-go Theorem for Lie-Hamilton systems [26] states that previous conditions ensure that $\mathcal{X}^H_{\mathcal{Q}}$ is not a Lie-Hamilton system.

A Dirac structure is a generalisation of presymplectic and Poisson structures, which can also be associated with Lie systems. Indeed, a Dirac structure on a manifold defines a foliation on it by presymplectic leaves in a similar way to the canonical foliation by symplectic leaves on any Poisson manifold. In particular, a presymplectic form on a manifold defines thus a Dirac structure on it. Hamiltonian vector fields on these Dirac structures are exactly the Hamilton vector fields of the structures originating them [29]. This fact makes possible to prove the following.

Corollary 1 *The Lie system $\mathcal{X}^H_{\mathcal{Q}}$ on $\mathcal{Q}$ determined by a quantum Lie system $H(t)$ is a Dirac-Lie system with respect to the Dirac structure induced by $\omega_{\mathcal{Q}}$.*

6.5.2 Lie Systems on the Manifold $\mathcal{R}$

The next results prove that the projection of the restriction of the Lie-Kähler system $\mathcal{X}^H$ to $M_{Q,0}$ onto $\mathcal{R}$ exists and it is a Lie-Hamilton system. It can be endowed with a natural coordinate system coming from this fact.

Lemma 1 *The manifold $\mathcal{R}$ admits a local coordinate system on a neighbourhood of each point given by the restrictions to $\mathcal{R}$ of $2n-1$ functions $f_\alpha(\psi) = \langle \psi, H_\alpha \psi \rangle$, for $\alpha = 1, 2, \ldots, 2n-1$, for certain traceless observables $H_\alpha \in \mathrm{Herm}(\mathcal{H})$.*

Proof For $n > 1$ any two elements of $M_{Q,0}$ with the same norm can be connected by the action of an element of $SU(n)$. Hence, the special unitary action $\varphi : SU(n) \times M_{Q,0} \to M_{Q,0}$, with $n > 1$, has $(2n-1)$-dimensional orbits, which are embedded submanifolds of $M_{Q,0}$. Since $\dim SU(n) = n^2 - 1 \geq 2n - 1$ for $n > 1$, there exists for any point of $M_{Q,0}$ an open neighbourhood A_0 containing it and where $2n-1$ fundamental vector fields of φ are linearly independent at each point. As they are also Hamiltonian vector fields, their Hamiltonian functions, which can be taken of the form $f_\alpha(\psi) = \langle \psi, H_\alpha \psi \rangle$, with $H_\alpha \in \mathrm{Herm}(\mathcal{H})$ being traceless observables and $\alpha = 1, 2, \ldots, 2n-1$, are functionally independent on A_0. These functions are invariant under the natural action of $U(1)$ on $M_{Q,0}$, and give rise to well-defined functions $f_1|_{\mathcal{R}}, \ldots, f_{2n-1}|_{\mathcal{R}}$, on an open subset of $\mathcal{R}$. As $f_1, \ldots, f_{2n-1}$ are functionally independent on $A_0 \subset M_{Q,0}$, then $f_1|_{\mathcal{R}}, \ldots, f_{2n-1}|_{\mathcal{R}}$ are functionally independent and provide a local coordinate system on $\mathcal{R}$.

Lemma 1 provides a method to define coordinate systems on the quantum quotient manifold $\mathcal{R}$ of any finite-dimensional quantum system. To illustrate this result, consider again the 2-level system described in Sect. 6.4.1. Hamiltonian functions h_1, h_2, h_3 defined in (6.32) satisfy the conditions of Lemma 1, hence they provide a coordinate system on $\mathcal{R}$ by

$$\begin{aligned} \phi_\sigma(\psi) = (h_1(\psi), h_2(\psi), h_3(\psi)) = (x_1, x_2, x_3) \in \mathbb{R}^3 \\ \Rightarrow \begin{cases} x_1 = q_1 q_2 + p_1 p_2 = 2\mathrm{Re}\,(z_1^* z_2), \\ x_2 = q_1 p_2 - q_2 p_1 = 2\mathrm{Im}\,(z_1^* z_2), \\ x_3 = \dfrac{1}{2}(q_1^2 + p_1^2 - q_2^2 - p_2^2) = (|z_1|^2 - |z_2|^2), \end{cases} \end{aligned} \tag{6.38}$$

with notation $(z_1, z_2) = (q_1 + \mathrm{i}p_1, q_2 + \mathrm{i}p_2)/\sqrt{2}$. Simple computations show that $\phi_\sigma^{-1}(x_1, x_2, x_3)$ is the equivalence class of an element of $\mathcal{R}$ for every $(x_1, x_2, x_3) \in \mathbb{R}^3_0$ and $\mathcal{R} \cong \mathbb{R}^3_0$.

Once defined an appropriate differentiable structure on the manifold $\mathcal{R}$, the following results show the properties of the Lie systems representing the t-dependent Schrödinger equation on this manifold.

Proposition 9 *The t-dependent Schrödinger equation, when restricted to $M_{Q,0}$, can be projected onto $\mathcal{R}$ originating a Lie-system $\mathcal{X}^H_{\mathcal{R}}$ possessing a Vessiot-Guldberg Lie algebra $V_{\mathcal{R}} \simeq \mathfrak{su}(\mathcal{H})$ of Hamiltonian vector fields with respect to the projection of Ω on $M_{Q,0}$ onto $\mathcal{R}$.*

Proof The $\mathbb{C}$-linear Lie group action $\varphi_M : U(\mathcal{H}) \times M_{Q,0} \to M_{Q,0}$ induces, due to its $\mathbb{C}$-linearity, an action $\phi_{\mathcal{R}}$ on $\mathcal{R}$ such that the map $\pi_{M\mathcal{R}}$ is equivariant, as follows:

$$\begin{aligned} \varphi_{\mathcal{R}} : U(\mathcal{H}) \times \mathcal{R} &\longrightarrow \mathcal{R}, \\ (g, [\psi]_{\mathcal{R}}) &\longmapsto [\varphi_M(g, \psi)]_{\mathcal{R}}. \end{aligned} \tag{6.39}$$

Let V_M denote the algebra of fundamental vector fields of φ_M. As a consequence of (6.39), vector fields in V_M project onto $\mathcal{R}$ giving rise to a new finite-dimensional Lie algebra of vector fields $V_{\mathcal{R}}$. The projection map $\pi_{M\mathcal{R}} : M_{Q,0} \to \mathcal{R}$ induces a Lie algebra morphism $\pi_{M\mathcal{R}*}|_{V_M} : V_M \to V_{\mathcal{R}}$. Then, the restriction to $M_{Q,0}$ of the Lie-Kähler system $\mathcal{X}^H$ describing Schrödinger equation also projects onto $\mathcal{R}$, giving rise to a Lie system $\mathcal{X}^H_{\mathcal{R}}$.

It can be proved that $\mathcal{X}^H_{\mathcal{R}}$ admits a Vessiot-Guldberg Lie algebra isomorphic to $\mathfrak{su}(\mathcal{H})$. As $V_M \simeq \mathfrak{u}(\mathcal{H}) \simeq \mathbb{R} \oplus \mathfrak{su}(\mathcal{H})$, the kernel of $\pi_{M\mathcal{R}*}|_{V_M}$, which is an ideal of V_M, may be either zero, isomorphic to $\mathbb{R}$, to $\mathfrak{su}(\mathcal{H})$ or to $\mathfrak{u}(\mathcal{H})$. The one-parameter group of diffeomorphisms induced by the vector field Γ is given by $\Phi^{\Gamma}_t : \psi \in M_{Q,0} \mapsto e^{it}\psi \in M_{Q,0}$. Hence, $\pi_{M\mathcal{R}*}(\Gamma) = 0$ and Γ belongs to the center of V_M. As $V_{\mathcal{R}} \neq 0$ and in view of the decomposition of V_M, then $\ker \pi_{M\mathcal{R}*} \simeq \langle \Gamma \rangle$ and $\operatorname{Im} \pi_{M\mathcal{R}*}|_{V_M} \simeq \mathfrak{su}(\mathcal{H})$. Thus, the projection of the Lie-Kähler system $\mathcal{X}^H$ onto $\mathcal{R}$ admits a Vessiot-Guldberg Lie algebra $V_{\mathcal{R}} \simeq \mathfrak{su}(\mathcal{H})$.

In the case of 2-level systems, a simple computation shows that there exist vector fields Y_α on $\mathcal{R}$ such that $\pi_{M\mathcal{R}*}(X_\alpha) = Y_\alpha$ for $\alpha = 1, 2, 3$. Indeed,

$$Y_1 = -2x_3\frac{\partial}{\partial x_2} + 2x_2\frac{\partial}{\partial x_3}, \quad Y_2 = 2x_3\frac{\partial}{\partial x_1} - 2x_1\frac{\partial}{\partial x_3}, \quad Y_3 = -2x_2\frac{\partial}{\partial x_1} + 2x_1\frac{\partial}{\partial x_2}. \tag{6.40}$$

The Lie brackets between these vector fields read

$$[Y_j, Y_k] = -2\sum_{l=1}^{3} \epsilon_{jkl} Y_l, \quad j, k = 1, 2, 3. \tag{6.41}$$

The projection of the Lie-Kähler system $\mathcal{X}^H$ given in (6.26) onto $\mathcal{R}$, i.e. the t-dependent vector field $\mathcal{X}^H_{\mathcal{R}}$ on $\mathcal{R}$ satisfying $(\mathcal{X}^H_{\mathcal{R}})_t = \pi_{M\mathcal{R}*}(X_t)$, becomes

$$\mathcal{X}^H_{\mathcal{R}} = \sum_{j=1}^{3} B_j(t) Y_j, \quad t \in \mathbb{R}. \tag{6.42}$$

The commutation relations in (6.41) show that the Vessiot-Guldberg Lie algebra of $\mathcal{X}^H_{\mathcal{R}}$ is isomorphic to $\mathrm{Herm}(2) \cong \mathfrak{su}^*(2)$. Therefore, $\mathcal{X}^H_{\mathcal{R}}$ is a Lie system.

Proposition 10 *The Lie system $\mathcal{X}^H_{\mathcal{R}}$ is a Lie-Hamilton system with respect to the bivector field $\pi_{M\mathcal{R}*}(\Omega)$, which is a Poisson tensor.*

Proof From formulas (6.12) and (6.14), one obtains that $\mathcal{L}_\Gamma \Omega = 0$ and therefore the Poisson bivector Ω on $M_{Q,0}$ can be projected onto $\mathcal{R}$. Additionally,

$$\pi_{M\mathcal{R}*}([\Omega, \Omega]_{SN}) = [\pi_{M\mathcal{R}*}(\Omega), \pi_{M\mathcal{R}*}(\Omega)]_{SN}, \tag{6.43}$$

with $[\cdot, \cdot]_{SN}$ being the Schouten-Nijenhuis bracket [52]. Thus, $\pi_{M\mathcal{R}*}(\Omega)$ is a Poisson bivector on $\mathcal{R}$. The vector fields X_α spanning the Vessiot-Guldberg Lie algebra V_M of $\mathcal{X}^H$ are Hamiltonian relative to the restrictions to $M_{Q,0}$ of the functions h_α in (6.32). Such Hamiltonian functions are invariant with respect to the action of $U(1)$ on $M_{Q,0}$ and hence projectable onto $\mathcal{R}$. The projections $\pi_{M\mathcal{R}*}(X_\alpha)$ are thus Hamiltonian vector fields with Hamiltonian functions $x_\alpha \in C^\infty(\mathcal{R})$ such that $h_\alpha = \pi^*_{M\mathcal{R}}(x_\alpha)$. Therefore, the Vessiot-Guldberg Lie algebra $V_\mathcal{R}$ on $\mathcal{R}$ consists of Hamiltonian vector fields relative to $\pi_{M\mathcal{R}*}(\Omega)$.

Proposition 11 *The Vessiot-Guldberg Lie algebra of the Lie system $\mathcal{X}^H_\mathcal{R}$ consists of Killing vector fields with respect to the metric induced by the projection of the tensor field G onto $\mathcal{R}$.*

Proof The tensor field G projects onto $\mathcal{R}$, as the Lie derivative of G with respect to Γ is zero. Since G comes from a Riemannian metric, it is non-degenerate, and so is its projection onto $\mathcal{R}$, giving rise to a Riemannian metric on $\mathcal{R}$. The vector fields of V_M are Killing relative to G and projectable under $\pi_{M\mathcal{R}*}$. Therefore, their projections, namely the elements of $V_\mathcal{R}$, are also Killing vector fields relative to the projection of G onto $\mathcal{R}$ and span a Vessiot-Guldberg Lie algebra $V_\mathcal{R}$ of Killing vector fields.

6.5.3 Lie-Kähler System on the Projective Manifold $\mathcal{P}$

As proved above, it is possible to project the Lie-Kähler system $\mathcal{X}^H$ associated with a quantum Lie system $H(t)$ onto the projective manifold $\mathcal{P}$. Additionally, we prove in this section that this manifold is endowed with a Kähler structure that is preserved under the evolution of $\mathcal{X}^H$. Thus, the t-dependent vector field representing the projective t-dependent Schrödinger equation happens to be again a Lie-Kähler system.

Lemma 2 *The Lie-Kähler system $\mathcal{X}^H$ on $M_{Q,0}$ related to a t-dependent Schrödinger equation is projectable under $\pi : M_{Q,0} \to \mathcal{P}$ onto a Lie system $\mathcal{X}^H_\mathcal{P}$.*

Proof Let $\varphi_M : U(\mathcal{H}) \times M_{Q,0} \to M_{Q,0}$ be the action the unitary group on $M_{Q,0}$. There exists a natural action of $U(\mathcal{H})$ onto $\mathcal{P}$ given by

$$\begin{aligned} \varphi_\mathcal{P} : U(\mathcal{H}) \times \mathcal{P} &\to \mathcal{P}, \\ (g, [\psi]_\mathcal{P}) &\mapsto [\varphi_M(g, \psi)]_\mathcal{P}. \end{aligned} \tag{6.44}$$

Then, the map $\pi : M_{Q,0} \to \mathcal{P}$ is equivariant relative to φ_M and $\varphi_\mathcal{P}$. Let V_M and $V_\mathcal{P}$ denote the Lie algebras of fundamental vector fields of φ_M and $\varphi_\mathcal{P}$, respectively.

Each vector field of V_M projects onto a fundamental vector field of $\varphi_{\mathcal{P}}$. As $\mathcal{X}^H$ takes values in V_M, this ensures $\mathcal{X}^H_{\mathcal{P},t} = \pi_*(\mathcal{X}^H_t)$ to exist for each $t \in \mathbb{R}$. Thus, $\mathcal{X}^H_{\mathcal{P}}$ is a Lie system whose Vessiot-Guldberg Lie algebra is $V_{\mathcal{P}}$.

Definition 6 Given a Schrödinger equation (6.24), with $\mathcal{X}^H$ being its corresponding Lie-Kähler system on M_Q, the *projective Schrödinger equation* on $\mathcal{P}$ is the system of differential equations

$$\frac{\mathrm{d}\xi}{\mathrm{d}t} = \mathcal{X}^H_{\mathcal{P}}(t, \xi), \quad \xi \in \mathcal{P}, \quad \forall t \in \mathbb{R}, \tag{6.45}$$

where $\mathcal{X}^H_{\mathcal{P}}$ is the projection onto $\mathcal{P}$ of $\mathcal{X}^H$ via $\pi : M_{Q,0} \to \mathcal{P}$.

Theorem 5 *The system* (6.45) *is a Lie-Kähler system with respect to the natural Kähler structure on* $\mathcal{P}$ *and a Vessiot-Guldberg Lie algebra isomorphic to* $\mathfrak{su}(\mathcal{H})$.

Proof In view of Theorem 4, the vector fields of V_M leave invariant G and Ω, i.e. $\mathcal{L}_X \Omega = \mathcal{L}_X G = 0$ for every $X \in V_M$. Since these vector fields are projectable onto $\mathcal{P}$ in virtue of Lemma 2, their projections span a Vessiot-Guldberg Lie algebra $V_{\mathcal{P}}$ for $\mathcal{X}^H_{\mathcal{P}}$ of Kähler vector fields relative to the natural Kähler structure on $\mathcal{P}$. The natural projection map $\pi : M_{Q,0} \to \mathcal{P}$ induces a Lie algebra morphism $\pi_*|_{V_M} : V_M \to V_{\mathcal{P}}$. As $V_M \simeq \mathfrak{u}(\mathcal{H}) \simeq \mathbb{R} \oplus \mathfrak{su}(\mathcal{H})$, the kernel of $\pi_*|_{V_M}$, which is an ideal of V_M, may be either zero, isomorphic to $\mathbb{R}$, to $\mathfrak{su}(\mathcal{H})$ or to $\mathfrak{u}(\mathcal{H})$. The one-parameter group of diffeomorphisms induced by the vector field Γ on $M_{Q,0}$ is given by $\Phi^{\Gamma}_t : \psi \in M_{Q,0} \mapsto e^{it}\psi \in M_{Q,0}$. Hence, $\pi_*(\Gamma) = 0$ and Γ belongs to the kernel. Since $V_{\mathcal{P}} \neq \{0\}$ and in view of the decomposition of V_M, then $\ker \pi_* \simeq \langle \Gamma \rangle$ and $\operatorname{Im} \pi_*|_{V_M} \simeq \mathfrak{su}(\mathcal{H})$. Thus, $V_{\mathcal{P}} \simeq \mathfrak{su}(\mathcal{H})$.

6.6 Superposition Rules for Schrödinger Equations

It has been proved in the preceding section that Schrödinger equations are a particular type of Lie systems. Thus, the tools developed for the study of Lie systems can be employed in order to describe quantum evolution. In particular, it is possible to devise superposition rules that give as a result the general solution to the Schrödinger equation, either on M_Q or on any of the quantum quotient manifolds.

6.6.1 Particular Solutions of the Schrödinger Equation

It is possible to determine, for each manifold, the necessary number of particular solutions in order to derive a superposition rule. The algorithm that gives the number of necessary particular solution has been presented in [6, 20], and described in Theorem 2. The aim of the present section is to apply this algorithm to Lie-Kähler systems defined on M_Q. In order to obtain an appropriate result, some physical considerations have to be made.

Due to the expression (6.25) of quantum Lie systems, the general Vessiot-Guldberg Lie algebra of a generic Lie-Kähler system on M_Q is isomorphic to $\mathcal{O} = \mathrm{Herm}(\mathcal{H})$. From a physical perspective, however, only vector fields with non-zero projection onto $\mathcal{P}$ are relevant. This is not the case of the Hamiltonian vector field X_I associated with the identity observable. This element, and any other proportional to it, is to be removed from the Vessiot-Guldberg algebra of the Lie-Kähler system. The result is isomorphic to the Lie algebra of traceless Hermitian operators on $\mathcal{H}$, which is itself isomorphic to $\mathfrak{su}(\mathcal{H})$. This is the Lie algebra of traceless skew-Hermitian operators on $\mathcal{H}$, and the Lie algebra associated with the Lie group $SU(\mathcal{H})$ of special unitary transformations on $\mathcal{H}$. Because of this physical property, an interesting result can be obtained, as seen next.

Theorem 6 *Every Lie-Kähler system $\mathcal{X}^H$ on M_Q with a traceless operator $H(t)$ admits a superposition rule depending on $n-1$ particular solutions.*

Proof Consider a traceless quantum Lie-system $H(t)$ on $\mathcal{H}$ and its corresponding Lie system $\mathcal{X}^H$ on M_Q. In view of Theorem 4, this system admits a Vessiot-Guldberg Lie algebra V^H of Kähler vector fields isomorphic to $\mathfrak{su}(\mathcal{H})$. The first step to derive a superposition rule is the determination of the smallest $m \in \mathbb{N}$ such that the diagonal prolongations to M_Q^m of the vector fields of V span a distribution of rank dim V at a generic point. The elements of V^H are fundamental vector fields of the standard linear action of $SU(\mathcal{H})$ on M_Q (thought of as a $\mathbb{C}$-linear space). The diagonal prolongations of V^H to M_Q^m span the tangent space to the orbits of the Lie group action

$$\begin{array}{rccc} \varphi_M^m : & SU(\mathcal{H}) \times M_Q^m & \longrightarrow & M_Q^m \\ & (U; \psi_1, \ldots, \psi_m) & \longmapsto & (U\psi_1, \ldots, U\psi_m). \end{array} \tag{6.46}$$

The fundamental vector fields of this action span a distribution of rank dim V at $\xi \in M_Q^m$ if and only if its isotropy group $\mathcal{O}_\xi$ at $\xi \in M_Q^m$ is discrete. With the hypothesis $m = n-1$, the elements $U \in \mathcal{O}_\xi$, with $\xi := (\psi_1, \ldots, \psi_{n-1}) \in M_Q^{n-1}$, satisfy

$$U\psi_j = \psi_j, \quad j = 1, 2, \ldots, n-1. \tag{6.47}$$

At a generic point of M_Q^{n-1}, the components $\psi_1, \ldots, \psi_{n-1}$ can be assumed to be linearly independent elements (over $\mathbb{C}$). Then, the knowledge of the action of U on these elements fixes U on $\langle \psi_1, \ldots, \psi_{n-1} \rangle_{\mathbb{C}} \subset M_Q$, where it acts as the identity map. If ψ is orthogonal to $\langle \psi_1, \ldots, \psi_{n-1} \rangle_{\mathbb{C}}$ with respect to the natural Hermitian product on $\mathcal{H}$, then $U\psi$ must also be orthogonal to $\langle \psi_1, \ldots, \psi_{n-1} \rangle_{\mathbb{C}}$ because of (6.47) and the unitarity of U. Therefore, $U\psi$ is proportional to ψ. Since $U \in SU(\mathcal{H})$ and $U\psi = \psi$, then $U = \mathrm{Id}$. Therefore, the isotropy group of φ^m is trivial at a generic point of M_Q^{n-1}, the fundamental vector fields of φ_M^m are linearly independent over $\mathbb{R}$ and there exists a superposition rule depending on $n-1$ particular solutions.

Remark 1 As $\mathcal{H}$ is a linear space and the Schrödinger equation is linear, there always exists a linear superposition rule for the Schrödinger equation depending on n par-

ticular solutions. Theorem 6 proves the existence of a different superposition rule, not necessarily linear, depending only on $n-1$ particular solutions.

It is worth noting that, if $m < n-1$, then the isotropy group for φ^m is not trivial at any point of M_Q^m. Given m linearly independent elements $(\psi_1, \ldots, \psi_m)$ over $\mathbb{C}$, there exist special unitary transformations on M_Q acting as the identity on $\langle \psi_1, \ldots, \psi_m \rangle_{\mathbb{C}}$ and leaving stable its orthogonal complement. Hence, the isotropy group on any point of M_Q^m is not discrete.

Since the elements of $U(\mathcal{H})$ act on M_Q preserving the norm relative to $\mathcal{H}$, the Lie group action φ_M^m given in the proof of the previous theorem can be restricted to $\mathcal{Q}^m$. In view of this, the previous proof can be slightly modified to prove that the restriction of φ_M^m to $\mathcal{Q}^m$ have a trivial isotropy group at a generic point for $m = n-1$. This proves the following corollary.

Corollary 2 *Every Lie system $\mathcal{X}_{\mathcal{Q}}^H$ on $\mathcal{Q}$ with a Vessiot-Guldberg Lie algebra $V^H \subset V_{\mathcal{Q}}$ isomorphic to $\mathfrak{su}(\mathcal{H})$ admits a superposition rule depending on $n-1$ particular solutions.*

Similar results can be proved for the Lie systems on the remaining quantum quotient manifold $\mathcal{R}$ and $\mathcal{P}$, as seen next.

Theorem 7 *Every Lie system $\mathcal{X}_{\mathcal{R}}^H$ on $\mathcal{R}$ admits a superposition rule depending on n particular solutions.*

Proof In view of Proposition 9, the Lie system $\mathcal{X}_{\mathcal{R}}^H$ admits a Vessiot-Guldberg Lie algebra $V_{\mathcal{R}}$ of fundamental vector fields isomorphic to $\mathfrak{su}(\mathcal{H})$. Also the proof of Proposition 9 shows that the diagonal prolongation of the elements of $V_{\mathcal{R}}$ to $\mathcal{R}^m$ are the fundamental vector fields of the Lie group action

$$\begin{array}{rccc} \varphi_{\mathcal{R}}^m : & SU(\mathcal{H}) \times \mathcal{R}^m & \to & \mathcal{R}^m \\ & (U; [\psi_1]_{\mathcal{R}}, \ldots, [\psi_m]_{\mathcal{R}}) & \mapsto & ([U\psi_1]_{\mathcal{R}}, \ldots, [U\psi_m]_{\mathcal{R}}). \end{array} \tag{6.48}$$

The derivation of a superposition rule for $\mathcal{X}_{\mathcal{R}}^H$ requires the determination of the necessary number m of particular solutions. This number is the smallest positive integer number such that the diagonal prolongations of the vector fields in $V_{\mathcal{R}}$ be linearly independent at a generic point. This occurs at $\xi \in \mathcal{R}^m$ if and only if the isotropy group of this action at ξ is discrete. If $m = n$, then the elements of the isotropy group of $\varphi_{\mathcal{R}}^n$ at a generic point $(\psi_1, \ldots, \psi_n) \in \mathcal{R}^n$ satisfy

$$U[\psi_j]_{\mathcal{R}} = [\psi_j]_{\mathcal{R}}, \quad j = 1, 2, \ldots, n. \tag{6.49}$$

At a generic point of $\mathcal{R}^n$, the elements $\psi_1, \ldots, \psi_n$ are linearly independent (over $\mathbb{C}$). In view of (6.48) and (6.49), the operator U diagonalises on the basis $\psi_1, \ldots, \psi_n$. In particular, the conditions (6.49) show that a fixed $U \in SU(\mathcal{H})$, which is acting on the elements $[\psi_j]_{\mathcal{R}}$, must satisfy that $U\psi_i = e^{\mathrm{i}\theta_i}\psi_i$ for certain $\theta_i \in [0, 2\pi[$. Since $U \in SU(\mathcal{H}) \subset U(\mathcal{H})$, then $\langle U\psi_i, U\psi_j \rangle = \langle \psi_i, \psi_j \rangle$ for $i, j = 1, 2, \ldots, n$. Hence, $e^{\mathrm{i}(\theta_j - \theta_i)} \langle \psi_i | \psi_j \rangle = \langle \psi_i | \psi_j \rangle$ for $i, j = 1, \ldots, n$. At a generic point, the elements

$\psi_1, \ldots, \psi_n$ are not orthogonal and therefore $\theta_i - \theta_j \in 2\pi\mathbb{Z}$ for all $i, j = 1, \ldots, n$. Thus, all factors in the diagonal of the matrix representation of U must be equal. As $U \in SU(\mathcal{H})$, the multiplication of such diagonal elements must be equal to 1. This fixes $U = e^{\mathrm{i}2\pi k/n}\mathrm{Id}_{\mathcal{H}}$ for $k \in \mathbb{Z}$. Therefore, the stability group of $\varphi^n_{\mathcal{R}}$ is discrete at a generic point of $\mathcal{R}^n$, the fundamental vector fields of $\varphi^n_{\mathcal{R}}$ are linearly independent over $\mathbb{R}$ at a generic point and $\mathcal{X}^H_{\mathcal{R}}$ admits a superposition rule depending on n particular solutions.

As presented in Fig. 6.2, the projective manifold $\mathcal{P}$ can be embedded naturally within $\mathcal{R}$. Additionally, the projection $\pi_{\mathcal{R}\mathcal{P}} : \mathcal{R} \to \mathcal{P}$ is equivariant relative to the the Lie group action of $SU(\mathcal{H})$ on $\mathcal{R}$ and the action $\varphi_{\mathcal{P}}$ of $SU(\mathcal{H})$ on $\mathcal{P}$. Following the same line of reasoning as in Corollary 2, the following result can be proved.

Corollary 3 *Every Lie-Kähler system on $\mathcal{P}$ admits a superposition rule depending on n particular solutions.*

6.6.2 Constants of Motion and Superposition Rules

The next step in order to obtain the superposition rules for Schrödinger equations is the computation of constants of motion. The characterisation of Lie systems on the relevant manifold makes this task easier. As shown next, it is possible to describe a general method so as to obtain constants of motion for Lie-Kähler systems. This method could have interesting applications in order to obtain solutions for the Schrödinger equation, as it can easily be implemented in numerical computations. Thus, Lie systems prove to be a powerful tool in the computation of the dynamics of quantum systems.

The superposition rule is derived through a number of constant of motions of the diagonal extension of the Lie system to M^n_Q. The number of necessary functions is equal to the dimension of the manifold M_Q. Thus, the superposition rule for the Schrödinger equation on M_Q is obtained in terms of $2n$ functions on M^n_Q. These functions are first integrals for the diagonal prolongation $\mathcal{X}^{H[n]}$, and hence for all the diagonal prolongations $X^{[n]}_\alpha$, with $\alpha = 1, 2, \ldots, r$, of the vector fields spanning the Vessiot-Guldberg Lie algebra of $\mathcal{X}^H$.

Lemma 3 *Consider the volume form $\Omega_{\mathcal{H}}$ on the complex Hilbert space $\mathcal{H}$ defined in the given coordinate system as*

$$\Omega_{\mathcal{H}} := \mathrm{d}z_1 \wedge \cdots \wedge \mathrm{d}z_n. \tag{6.50}$$

Let Ω_R, Ω_I be the n-forms on M_Q defined as in terms of the real and imaginary parts of $\Omega_{\mathcal{H}}$:

$$\begin{aligned} (\Omega_R)_\psi(v_1, \ldots, v_n) &:= \sqrt{2^n} n \,\mathrm{Re}\, \Omega_{\mathcal{H}}(|v_1\rangle, \ldots, |v_n\rangle), \\ (\Omega_I)_\psi(v_1, \ldots, v_n) &:= \sqrt{2^n} n \,\mathrm{Im}\, \Omega_{\mathcal{H}}(|v_1\rangle, \ldots, |v_n\rangle), \end{aligned} \tag{6.51}$$

for any $\psi \in M_Q$ and any set $v_1, \ldots, v_n \in T_\psi M_Q$. These n-forms are invariants of Lie-Kähler systems associated with traceless quantum Lie systems.

Proof The value of $\Omega_{\mathcal{H}}$ on a set of tangent vectors $|\psi^1\rangle, \ldots, |\psi^n\rangle \in T_\psi \mathcal{H}$ can be directly computed by the determinant of their coordinates as $\Omega_{\mathcal{H}}(|\psi^1\rangle, \ldots, |\psi^n\rangle) = \det\left(\psi_k^j\right)$, with $\psi_1^j, \ldots, \psi_n^j \in \mathbb{C}$ the coordinates of $|\psi^j\rangle$ in the given basis, for $j = 1, 2, \ldots, n$. Then, as

$$\begin{aligned}\Omega_{\mathcal{H}}(e^{-\mathrm{i}tH}|\psi^1\rangle, \ldots, e^{-\mathrm{i}tH}|\psi^n\rangle) &= \mathrm{Det}\,(e^{-\mathrm{i}tH})\Omega_{\mathcal{H}}(|\psi^1\rangle, \ldots, |\psi^n\rangle)\\ &= e^{-\mathrm{i}t\mathrm{Tr}H}\,\Omega_{\mathcal{H}}(|\psi^1\rangle, \ldots, |\psi^n\rangle),\end{aligned} \tag{6.52}$$

the volume form is invariant for any traceless Hamiltonian H.

Lemma 4 *The functions $I_1^c, I_1^s, \ldots, I_n^c, I_n^s : (M_Q)^n \to \mathbb{R}$ defined at the point $(\psi^{(0)}, \ldots, \psi^{(n-1)})$ as*

$$\begin{aligned}
I_j^c &:= g^{[n]}(\Delta^{(0)}, S_{0j}(\Delta^{(j)})) = \sum_{k=1}^{n}(q_k^{(0)}q_k^{(j)} + p_k^{(0)}p_k^{(j)}), \qquad j = 1, \ldots, n-1;\\
I_j^s &:= g^{[n]}(\Gamma^{(0)}, S_{0j}(\Delta^{(j)})) = \sum_{k=1}^{n}(q_k^{(0)}p_k^{(j)} - p_k^{(0)}q_k^{(j)}),\\
I_n^c &:= \Omega_R^{[n]}\left(\Delta^{(0)}, S_{01}(\Delta^{(1)}), \ldots, S_{0(n-1)}(\Delta^{(n-1)})\right) = \sqrt{2^n}\,n\,\mathrm{Re}(\det(\psi^{(0)}, \ldots, \psi^{(n-1)})),\\
I_n^s &:= \Omega_I^{[n]}\left(\Delta^{(0)}, S_{01}(\Delta^{(1)}), \ldots, S_{0(n-1)}(\Delta^{(n-1)})\right) = \sqrt{2^n}\,n\,\mathrm{Im}(\det(\psi^{(0)}, \ldots, \psi^{(n-1)})),
\end{aligned} \tag{6.53}$$

with S_{rs} being the (1,1)-tensor field on M_Q^n that interchanges components r, s of vector fields on the product manifold, i.e. $T\pi_r(S_{rs}X) = T\pi_s(X)$, for any vector field X on M_Q^n, π_k representing the canonical projection on the k–th component of the product manifold, are constants of motion for the diagonal prolongation $\mathcal{X}^{H[n]}$ of the Lie-Kähler system $\mathcal{X}^H$ on M_Q defined by a traceless quantum Lie system $H(t)$. These functions satisfy the relations

$$(J^{(j)} - J^{(0)})(\mathrm{d}I_j^c) = \mathrm{d}I_j^s, \qquad j = 1, 2, \ldots, n, \tag{6.54}$$

where $J^{(k)}$ represents the complex structure tensor corresponding to the k–th copy of M_Q^n and the matrix of partial derivatives of these functions is regular:

$$\det\left(\frac{\partial I_j}{\partial \xi_k^{(0)}}\right) \neq 0, \quad \textit{with } I = (I_j^c, I_j^s),\ \xi^{(0)} = (q_j^{(0)}, p_j^{(0)}). \tag{6.55}$$

Proof The Lie-Kähler system is decomposed as in (6.26). The vector fields $X_1, \ldots, X_r$ are Kähler vector fields relative to the Kähler structure (g, ω, J) on M_Q. Therefore, their diagonal prolongations $X_\alpha^{[n]}$ are Kähler relative to the diagonal prolongation $(g^{[n]}, \omega^{[n]}, J^{[n]})$ to $(M_Q)^n$ of the Kähler structure (g, ω, J).

Similarly, if X is a Hamiltonian vector field relative to ω with Hamiltonian function h_X, then $X^{[n]}$ is a Hamiltonian vector field with Hamiltonian function $h_X^{[n]}$. As the vector fields $X_1^{[n]}, \ldots, X_m^{[n]}$ are Killing vector fields with respect to $g^{[n]}$ and Lie symmetries of the tensor fields S_{rs} for $r, s = 0, 1, 2, \ldots, n-1$ and $r \neq s$, the functions I_j^c, I_j^s for $j = 1, \ldots, n-1$ are first integrals for the $X_1^{[n]}, \ldots, X_m^{[n]}$ and therefore they are constants of motion for $\mathcal{X}^{H[n]}$. As $(g^{[n]}, \omega^{[n]}, J^{[n]})$ conforms a Kähler structure, the functions satisfy by definition the relation $(J^{(k)} - J^{(0)})(\mathrm{d}I_k^c) = \mathrm{d}I_k^s$, for $k = 1, \ldots, n-1$. Observe that these functions are first-integrals not only for $X_\alpha^{[n]}$, but also for $\Gamma^{[n]}$.

As the vector fields $X_\alpha^{[n]}$ are Kähler, then I_n^c, I_n^s are first integrals of these vector fields and they are also constants of motion of $\mathcal{X}^{H[n]}$. It is worth noting that since the one-parameter group of diffeomorphisms of $\Gamma^{[n]}$ is given by the multiplication action of $U(1)$ on M_Q, the functions I_n^c and I_n^s are not invariant under these multiplications and such functions are not first-integrals of $\Gamma^{[n]}$.

It remains to be proved that the determinant (6.55) of the matrix of derivatives with respect to $q_1^{(0)}, p_1^{(0)}, \ldots, q_n^{(0)}, p_n^{(0)}$ is not zero. Observe that the pairs of functions (I_j^c, I_j^s) and $(I_{j'}^c, I_{j'}^s)$, with $j, j' = 1, 2, \ldots, n$, depend on different variables if $j \neq j'$, so their derivatives are functionally independent functions. Also, the relation $(J^{(n)} - J^{(0)})(\mathrm{d}I_n^c) = \mathrm{d}I_n^s$ proves that I_j^c and I_j^s are functionally independent for any $j = 1, 2, \ldots, n$. Thus, the determinant (6.55) cannot vanish (at a generic point).

Hence we can define these constants of the motion as a local chart for M_Q^n. Consider thus, with the functions defined in (6.53), the following system of equations:

$$\begin{cases} I_j^c(\psi^{(0)}, \psi^{(1)}, \ldots \psi^{(n-1)}) = k_{2j-1}, \\ I_j^s(\psi^{(0)}, \psi^{(1)}, \ldots \psi^{(n-1)}) = k_{2j}, \end{cases} \qquad j = 1, 2, \ldots, n. \tag{6.56}$$

The solution $\psi^{(0)}$ to the system can be obtained, at least locally, in terms of the coordinates of $\psi^{(1)}$, …, $\psi^{(n-1)}$ and $2n$ real constants k_1, …, k_{2n}. In other words, Lemma 4, in particular equation (6.54), guarantees that the functions are functionally independent and the system (6.56) can be solved locally for $\psi^{(0)}$.

A non-linear superposition rule for the Schrödinger equation on M_Q depending on $n-1$ particular solutions has thus been obtained. This applies to the case when the Schrödinger equation is determined by a t-dependent traceless Hamiltonian. The superposition rule can be derived from the constants of motion computed on M_Q^n for the diagonal prolongation $\mathcal{X}^{H[n]}$ of the Lie-Kähler system $\mathcal{X}^H$. It is possible to obtain an analytic result because of the simple expression of the constants of the motion as functions of the coordinates of M_Q. A similar procedure could be carried out in the projective manifold $\mathcal{P}$, as it also has a Kähler structure. However, a general result as the one presented above would be, at least, much more complicated. This is due to $\mathcal{P}$ lacking a global chart. Therefore, it will not be computed for the general case. Nevertheless, it is possible to derive a superposition rule for simple cases.

It is to be remarked that the process of superposition of two states in Quantum Mechanics has been studied from a geometric point of view by different authors

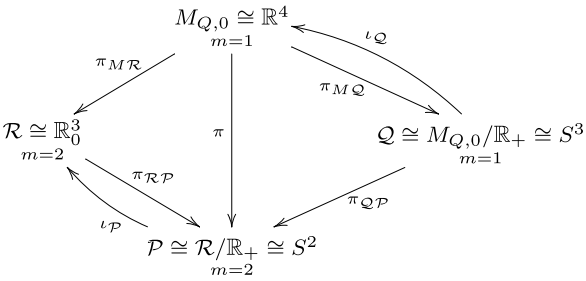

Fig. 6.3 Diagram of the differentiable manifolds appearing in the study of 2-level quantum systems. The number m under each manifold represents the number of particular solutions of the Schrödinger equation determining the general solution

(see [53–56]). Our goal in this paper is different, since we are finding a rule for the superposition of solutions of the Schrödinger equation, giving rise to its general solution. In the following Section, we illustrate the construction for a simple 2-level system.

6.7 Superposition Rules for 2-Level Systems

This section illustrates the theory presented in the previous section by describing superposition rules for 2-level systems on M_Q and on the quantum quotient manifolds. Recall the existing commutative diagram presented in Fig. 6.2. The diagram is reproduced in Fig. 6.3, where under each space the smallest number of particular solutions for its corresponding superposition rule appears.

On each space, there exists a Lie system admitting a Vessiot-Guldberg Lie algebra of Hamiltonian vector fields relative to different compatible geometric structures, which in turn makes possible to obtain, in a geometric way, their superposition rules. The following subsections provide these superposition rules, their relevant geometric properties and their potential applications in Quantum Mechanics.

6.7.1 Superposition Rule for a 2-Level System on M_Q and $\mathcal{Q}$

Consider a t-dependent vector field $\mathcal{X}^H$ on M_Q of the form

$$\mathcal{X}^H_t = \sum_{j=1}^{3} B_j(t) X_j, \quad t \in \mathbb{R}. \tag{6.57}$$

It is an immediate consequence of Theorem 4 that $\mathcal{X}^H$ is a Lie-Kähler system whose Vessiot-Guldberg Lie algebra $V = \langle X_1, X_2, X_3 \rangle$, with X_1, X_2, X_3 given by (6.30),

consists of Kähler vector fields relative to the standard Kähler structure (g, ω, J) on M_Q. Also, $\mathcal{X}_t^H$ commutes for any $t \in \mathbb{R}$ with the phase change vector field Γ and with the dilation vector field Δ, namely Γ and Δ are Lie symmetries of $\mathcal{X}^H$.

The superposition rule for $\mathcal{X}^H$ depends on a number m of particular solutions, which is the smallest integer such that the diagonal prolongations to $M_Q^m \simeq \left(\mathbb{R}^4\right)^m$ of X_1, X_2, X_3 are linearly independent at a generic point [6]. The coordinate expressions for X_1, X_2, X_3, given in (6.30), show that they are already linearly independent at a generic point of M_Q. Hence $m = 1$, i.e. the superposition rule does depend on a mere particular solution. This is a lower number than in the case of the standard quantum linear superposition rule, which depends on two particular solutions.

The functions that determine the superposition rule are given by Lemma 4:

$$\begin{aligned}
I_1^c(\psi^{(0)}, \psi^{(1)}) &:= g^{[2]}(\Delta^{(0)}, S_{01}\Delta^{(1)}) = q_1^{(0)}q_1^{(1)} + p_1^{(0)}p_1^{(1)} + q_2^{(0)}q_2^{(1)} + p_2^{(0)}p_2^{(1)},\\
I_1^s(\psi^{(0)}, \psi^{(1)}) &:= \omega^{[2]}(\Delta^{(0)}, S_{01}\Delta^{(1)}) = q_1^{(0)}p_1^{(1)} - p_1^{(0)}q_1^{(1)} + q_2^{(0)}p_2^{(1)} - p_2^{(0)}q_2^{(1)},\\
I_2^c(\psi^{(0)}, \psi^{(1)}) &:= \Omega_R^{[2]}(\Delta^{(0)}, S_{01}\Delta^{(1)}) = q_1^{(0)}q_2^{(1)} - p_1^{(0)}p_2^{(1)} - q_2^{(0)}q_1^{(1)} + p_2^{(0)}p_1^{(1)},\\
I_2^s(\psi^{(0)}, \psi^{(1)}) &:= \Omega_I^{[2]}(\Delta^{(0)}, S_{01}\Delta^{(1)}) = q_1^{(0)}p_2^{(1)} + p_1^{(0)}q_2^{(1)} - q_2^{(0)}p_1^{(1)} - p_2^{(0)}q_1^{(1)}.
\end{aligned} \tag{6.58}$$

These functions are first integrals for the diagonal prolongations $X_1^{[2]}, X_2^{[2]}, X_3^{[2]}$ of X_1, X_2, X_3 to $M_Q^2 \simeq (\mathbb{R}_0^4)^2$. The matrix of derivatives $\left(\frac{\partial I}{\partial \psi^{(0)}}\right)$ given in (6.54) is easily computed, and it is found to be regular in M_Q except for $(0, 0, 0, 0)$. It is thus possible to obtain a superposition rule by solving the system of equations $I_j^c(\psi^{(0)}, \psi^{(1)}) = k_j$, for $j = 1, 2, 3, 4$. The non-linear superposition rule in M_Q is

$$\begin{pmatrix} q_1^{(0)} \\ p_1^{(0)} \\ q_2^{(0)} \\ p_2^{(0)} \end{pmatrix} = \left(\frac{\partial I}{\partial \psi^{(0)}}\right)^{-1} \begin{pmatrix} k_1 \\ k_2 \\ k_3 \\ k_4 \end{pmatrix} = \frac{1}{\|\psi^{(1)}\|^2} \begin{pmatrix} q_1^{(1)} & p_1^{(1)} & q_2^{(1)} & p_2^{(1)} \\ p_1^{(1)} & -q_1^{(1)} & -p_2^{(1)} & q_2^{(1)} \\ q_2^{(1)} & p_2^{(1)} & -q_1^{(1)} & -p_1^{(1)} \\ p_2^{(1)} & -q_2^{(1)} & p_1^{(1)} & -q_1^{(1)} \end{pmatrix} \begin{pmatrix} k_1 \\ k_2 \\ k_3 \\ k_4 \end{pmatrix}. \tag{6.59}$$

It is possible to further simplify this expression. Its non-linearity is a consequence of the denominator. As proved several times in the preceding sections, the norm of states is preserved under the evolution due to the unitarity of Schrödinger equations. Thus, the constants k_1, k_2, k_3, k_4 can be replaced by new numbers that incorporate this factor. By defining the numbers

$$c_j = \frac{k_j}{(q_1^{(0)})^2 + (q_2^{(0)})^2 + (p_1^{(0)})^2 + (p_2^{(0)})^2}, \quad j = 1, 2, 3, 4, \tag{6.60}$$

expression (6.59) can be rewritten and, after some computations, the following theorem can be proved.

Theorem 8 *There exists a superposition rule for the Lie-Kähler system $\mathcal{X}^H$ on M_Q of the 2-level system, given on (6.57), depending on a single particular solution. The superposition rule*

$$\begin{aligned} \Phi : M_Q \times M_Q &\to M_Q \\ (\psi^{(1)}, c) &\mapsto \psi^{(0)}, \end{aligned} \tag{6.61}$$

can be given the following coordinate expression:

$$\begin{pmatrix} q_1^{(0)} \\ p_1^{(0)} \\ q_2^{(0)} \\ p_2^{(0)} \end{pmatrix} = \begin{pmatrix} c_1 & c_2 & c_3 & c_4 \\ -c_2 & c_1 & c_4 & -c_3 \\ -c_3 & -c_4 & c_1 & c_2 \\ -c_4 & c_3 & -c_2 & c_1 \end{pmatrix} \begin{pmatrix} q_1^{(1)} \\ p_1^{(1)} \\ q_2^{(1)} \\ p_2^{(1)} \end{pmatrix}. \tag{6.62}$$

Consider the projection $\pi_{MQ} : M_{Q,0} \to \mathcal{Q}$ and the natural embedding $\iota_{\mathcal{Q}} : \mathcal{Q} \to M_{Q,0}$ defined in Sect. 6.5. The Lie-Kähler system $\mathcal{X}^H$ can be projected through π_{MQ} onto a system $\mathcal{X}^H_{\mathcal{Q}}$ on $\mathcal{Q}$, as in Proposition 8. The superposition rule for $\mathcal{X}^H_{\mathcal{Q}}$ can be obtained from of the superposition for $\mathcal{X}^H$. Observe that $\mathcal{X}^H$ is a Lie system on $M_{Q,0}$ with a superposition rule $\Phi : M_{Q,0} \times M_{Q,0} \to M_{Q,0}$ and that $\mathcal{X}^H_t$ is tangent to the submanifold $\iota_{\mathcal{Q}}(\mathcal{Q}) \subset M_{Q,0}$ for each $t \in \mathbb{R}$. Assume also that there exists $\bar{S} \subset M_{Q,0}$ such that $\Phi(\mathcal{Q} \times \bar{S}) = \mathcal{Q}$. Then, the initial superposition rule can be restricted to elements on $\mathcal{Q}$ giving rise to a new superposition principle.

Indeed, the superposition rule Φ is defined in Theorem 8 and evaluated on points $\psi^{(1)}_{\mathcal{Q}}, c_{\mathcal{Q}} \in \mathcal{Q}$, i.e. $\|\psi^{(1)}_{\mathcal{Q}}\| = \|c_{\mathcal{Q}}\| = 1$. The resulting point $\Phi(\psi^{(1)}_{\mathcal{Q}}, c_{\mathcal{Q}})$ satisfies that

$$\|\Phi(\psi^{(1)}_{\mathcal{Q}}, c_{\mathcal{Q}})\| = \|c_{\mathcal{Q}}\|^4 \|\psi^{(1)}_{\mathcal{Q}}\| = 1 \Rightarrow \Phi(\psi^{(1)}_{\mathcal{Q}}, c_{\mathcal{Q}}) \in \mathcal{Q}.$$

Conversely, there always exists, for points $\psi^{(0)}_{\mathcal{Q}} \in \mathcal{Q}$ and $c_{\mathcal{Q}} \in \mathcal{Q}$, a point $\psi^{(1)}_{\mathcal{Q}} \in \mathcal{Q}$ such that $\Phi(\psi^{(1)}_{\mathcal{Q}}, c_s) = \psi^{(0)}_{\mathcal{Q}}$. Hence $X_{\mathcal{Q}}$ admits a superposition rule $\Phi_{\mathcal{Q}} : \mathcal{Q} \times \mathcal{Q} \to \mathcal{Q}$ which can be formally written as (6.62).

6.7.2 *Superposition Rules for the 2-Level System on $\mathcal{R}$ and $\mathcal{P}$*

The procedure developed for the Lie-Kähler system can be repeated in order to obtain a superposition rule on the quotient manifold $\mathcal{R}$. In particular, the 2-level system is a simple example in which the superposition rule can be written explicitly.

Recall from Lemma 1 that there exists a way to obtain coordinate systems in $\mathcal{R}$. In the case of 2-level systems, there exists a global chart with coordinates x, y, z, as given by (6.38). A Lie system $\mathcal{X}^H_{\mathcal{R}}$ on $\mathcal{R}$ determined by a quantum Lie system $H(t)$ can be written as

$$\mathcal{X}^H_{\mathcal{R},t} = \sum_{j=1}^{3} B_j(t) Y_j, \tag{6.63}$$

where Y_1, Y_2, Y_3 are given by (6.40). The superposition rule for $\mathcal{X}^H_{\mathcal{R}}$ depends on m particular solutions, where m is the smallest integer such that the diagonal prolon-

gations $Y_1^{[m]}, Y_2^{[m]}, Y_3^{[m]}$ to $\mathcal{R}^m$ are linearly independent at a generic point. Observe that Y_1, Y_2, and Y_3 span a two-dimensional distribution on $\mathcal{R}$. As the diagonal prolongations enlarge the dimensions of the distributions, it is enough to consider $\mathcal{R}^2$ to obtain linearly independent vectors at generic points, hence $m = 2$ (see [6, 20]).

The superposition rule is obtained by computing constants of motion of the diagonal prolongation of $\mathcal{X}_{\mathcal{R}}^H$ to $\mathcal{R}^3$. From the geometric properties of $\mathcal{X}_{\mathcal{R}}^H$ it is possible to obtain constants of motion $\hat{I}_1, \hat{I}_2, \hat{I}_3 : \mathcal{R}^3 \to \mathbb{R}$ as

$$\begin{aligned}
\hat{I}_1(\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}) &:= 2g_{\mathcal{R}}^{[3]}(\Delta^{(0)}, S_{01}\Delta^{(1)}) = \frac{x^{(0)}x^{(1)} + y^{(0)}y^{(1)} + z^{(0)}z^{(1)}}{\|\mathbf{x}^{(0)}\|}, \\
\hat{I}_2(\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}) &:= 2g_{\mathcal{R}}^{[3]}(\Delta^{(0)}, S_{02}\Delta^{(1)}) = \frac{x^{(0)}x^{(2)} + y^{(0)}y^{(2)} + z^{(0)}z^{(2)}}{\|\mathbf{x}^{(0)}\|}, \\
\hat{I}_3(\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}) &:= 2g_{\mathcal{R}}^{[3]}(\Delta^{(0)}, \Delta^{(0)}) = \|\mathbf{x}^{(0)}\|,
\end{aligned} \tag{6.64}$$

where $\mathbf{x}^{(j)} \in \mathcal{R}$ denotes a point with coordinates $(x^{(j)}, y^{(j)}, z^{(j)}) \in \mathbb{R}^3$, with $j = 0, 1, 2$, and the norm in $\mathcal{R}$ has the expression $\|\mathbf{x}\| = \sqrt{x^2 + y^2 + z^2}$.

As the considered vector fields are Killing with respect to the metric, norms are preserved. Thus, it is possible to obtain new constants of motion I_1, I_2, I_3 simply by multiplying functions in (6.64) by the norm $\|\mathbf{x}^{(0)}\|$. The matrix of derivatives of these functions is

$$\left(\frac{\partial I}{\partial \mathbf{x}^{(0)}}\right) = \begin{pmatrix} x^{(1)} & y^{(1)} & z^{(1)} \\ x^{(2)} & y^{(2)} & z^{(2)} \\ 2x^{(0)} & 2y^{(0)} & 2z^{(0)} \end{pmatrix}, \quad \det\left(\frac{\partial I}{\partial \mathbf{x}^{(0)}}\right) = 2\mathbf{x}^{(0)} \cdot \left(\mathbf{x}^{(1)} \times \mathbf{x}^{(2)}\right), \tag{6.65}$$

This shows that the matrix is regular if $\mathbf{x}^{(0)}, \mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$ are linearly independent. In this expression and the following, it is useful to use the vector notation that is common in $\mathbb{R}^3$. Thus, $\mathbf{x} \cdot \mathbf{y}$ and $\mathbf{x} \times \mathbf{y}$ denote respectively the scalar and vector product of vectors in $\mathbb{R}^3$.

Consider the system of equations $I_j = k_j$ for $j = 1, 2, 3$, with $k_3 > 0$. Solving for $\mathbf{x}^{(0)}$, the superposition rule for the Lie system $\mathcal{X}_{\mathcal{R}}^H$ is obtained. Observe that the system of equations can be rewritten as a set of three vector equations in $\mathbb{R}^3$:

$$\mathbf{x} \cdot \mathbf{x}_1 = k_1, \qquad \mathbf{x} \cdot \mathbf{x}_2 = k_2, \qquad \mathbf{x} \cdot \mathbf{x} = k_3, \qquad k_1, k_2, k_3 \in \mathbb{R},\ k_3 > 0. \tag{6.66}$$

Since $\mathbf{x}_1$ and $\mathbf{x}_2$ are not collinear when the matrix (6.65) is regular, these vectors together with $\mathbf{x}_1 \times \mathbf{x}_2$ conform an orthonormal basis for $\mathbb{R}^3$. From (6.66), the general expression for $\mathbf{x}$ is

$$\mathbf{x} = \frac{\delta_{12}\mathbf{x}_1 + \delta_{21}\mathbf{x}_2 \pm \sqrt{k_3[\|\mathbf{x}_1\|^2\|\mathbf{x}_2\|^2 - (\mathbf{x}_1 \cdot \mathbf{x}_2)^2] - (k_1\mathbf{x}_1 - k_2\mathbf{x}_2)^2}\, \mathbf{x}_1 \times \mathbf{x}_2}{\|\mathbf{x}_1\|^2\|\mathbf{x}_2\|^2 - (\mathbf{x}_1 \cdot \mathbf{x}_2)^2},$$

where $\delta_{lj} := k_l \|\mathbf{x}_j\|^2 - k_j(\mathbf{x}_l \cdot \mathbf{x}_j)$. As the Lie system $\mathcal{X}^H_{\mathcal{R}}$ is linear in the chosen coordinate system and the Riemannian metric related to the standard scalar product on $\mathcal{R}$ is invariant under the elements of $V_{\mathcal{R}}$, it follows that $\|\mathbf{x}_1\|^2$, $\|\mathbf{x}_2\|^2$ and $\mathbf{x}_1 \cdot \mathbf{x}_2$ are constant along particular solutions of $\mathcal{X}^H_{\mathcal{R}}$. It is thus possible to simplify the expression, leading to the following results.

Theorem 9 *The superposition rule for the Lie system $\mathcal{X}^H_{\mathcal{R}}$ on $\mathcal{R}$ is a function $\Phi_{\mathcal{R}} : \mathcal{R}^2 \times \mathcal{A} \to \mathcal{R}$ with $A := \{(k_1, k_2, k_3) \in \mathbb{R}^3 : k_3 > 0\}$, given by*

$$\Phi_{\mathcal{R}}(\mathbf{x}_1, \mathbf{x}_2, (k_1, k_2, k_3)) = \delta_{12}\mathbf{x}_1 + \delta_{21}\mathbf{x}_2 + \sqrt{k_3 k_{12} - (k_1\mathbf{x}_1 - k_2\mathbf{x}_2)^2}\, \mathbf{x}_1 \times \mathbf{x}_2, \tag{6.67}$$

where $k_{12} := \|\mathbf{x}_1\|^2\|\mathbf{x}_2\|^2 - (\mathbf{x}_1 \cdot \mathbf{x}_2)^2$.

To obtain the superposition rule for the system $\mathcal{X}^H_{\mathcal{P}}$ on $\mathcal{P}$, consider the natural embedding of $\mathcal{P}$ into $\mathcal{R}$ whose image is the set of elements $(x, y, z) \in \mathcal{R}$ such that $x^2 + y^2 + z^2 = 1$. Therefore, $\mathcal{P}$ is diffeomorphic to a sphere $S^2 \subset \mathcal{R} \simeq \mathbb{R}^3_0$. The superposition rule defined for $\mathcal{X}^H_{\mathcal{R}}$ should be restricted to points in S^2, i.e. with $\|\mathbf{x}_1\| = \|\mathbf{x}_2\| = 1$. In consequence, constants have to be constrained as $|k_1|, |k_2| \leq 1$, $k_3 = 1$, and the superposition rule for $\mathcal{P}$ can be written in terms of its embedding into $\mathcal{R}$ as

$$\mathbf{x} = \delta_{12}\mathbf{x}_1 + \delta_{21}\mathbf{x}_2 + \sqrt{k_{12} - (k_1\mathbf{x}_1 - k_2\mathbf{x}_2)^2}\, \mathbf{x}_1 \times \mathbf{x}_2, \quad \mathbf{x}_1, \mathbf{x}_2 \in \mathcal{P}, \quad |k_1|, |k_2| \leq 1. \tag{6.68}$$

where $k_{12} := 1 - (\mathbf{x}_1 \cdot \mathbf{x}_2)^2$ and $\delta_{lj} := k_l - k_j(\mathbf{x}_l \cdot \mathbf{x}_j)$, for $j, l = 1, 2$.

6.8 Conclusions and Outlook

Systems of differential equations appear in every description of Quantum Mechanics. Thus, it is indubitable that any method of resolution has great importance in Physics. Lie systems offer a new perspective in this topic. As proved along this work, the geometric formalism offers a suitable framework for the application of this tool. Thus, it is possible to solve the Schrödinger equation for finite-dimensional systems by means of a superposition rule, at the level of the Hilbert space, but also at any of the possible quantum quotient manifolds $\mathcal{Q}, \mathcal{R}$ and $\mathcal{P}$. Thus, Lie systems and superposition rules are a powerful tool to describe dynamics on these manifolds. This is very relevant, as the common algebraic description of Quantum Mechanics usually ignores the different geometric structures.

It is remarkable that the superposition rules obtained in this work are nonlinear. Schrödinger equation, as a linear differentiable equation on a Hilbert space, naturally carries a linear superposition rule. The approach presented in this work, however, yields a different result. As seen in Sect. 6.6.2, Schrödinger equations on M_Q determined by traceless t-dependent Hamiltonians can be solved by means of a generally non-linear superposition rule depending on less particular solutions than the standard

linear superposition rule. Indeed, as the Lie systems on M_Q and $\mathcal{P}$ are associated with the same group, and $\mathcal{P}$ is no longer linear and encodes the "true" quantum degrees of freedom of the system, it is not surprising that the associated Lie system on M_Q also captures part of these nonlinear properties. A detailed analysis of the general properties of the superposition rules on the different quotient manifolds may also help to obtain more information about these issues and will be covered in future works.

Acknowledgements J. F. Cariñena, J. A. Jover-Galtier and J. Clemente-Gallardo acknowledge partial financial support from MINECO (Spain) grant number MTM2015-64166-C2-1. Research of J. de Lucas was supported under the contract 1100/112000/16. Research of J. Clemente-Gallardo and J. A. Jover-Galtier was financed by projects MICINN Grants FIS2013-46159-C3-2-P. Research of J. A. Jover-Galtier was financed by DGA grant number B100/13 and by "Programa de FPU del Ministerio de Educación, Cultura y Deporte" grant number FPU13/01587.

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Chapter 7
Killing Vector Fields and Quantisation of Natural Hamiltonians

José F. Cariñena, Manuel F. Rañada and Mariano Santander

Abstract The usual canonical prescription ordinarily made for the obtention of the quantum Hamiltonian operator for a classical system leads to some ambiguities in situations beyond the simplest ones and these ambiguities arise unavoidably when the configuration space is not Euclidean and in systems in Euclidean space with a position-dependent mass. A recently proposed method to circumvent this difficulty for natural Hamiltonians will be described. The idea is not to quantise the coordinates and their (classical) conjugate momenta (which is where the ambiguities could arise), but to work directly with Killing vector fields and associated Noether momenta in order to get in some unambiguous way the corresponding Hamiltonian operator. The example of one-dimensional position-dependent mass systems and in particular the motion along a regular curve, both in the classical and the quantum case, is analysed and is illustrated with the case of quantum motion on a cycloid. As another example, the motions on constant curvature surfaces will be used to illustrate the method. In both examples it is crucial the choice as Hilbert space the linear space of square integrable functions, satisfying appropriate boundary conditions, with respect to the measure that is invariant under the Killing vector field.

AMS Classification 70S05 · 81Q70

J. F. Cariñena (✉) · M. F. Rañada
Departamento de Física Teórica and IUMA, Facultad de Ciencias,
Universidad de Zaragoza, 50009 Zaragoza, Spain
e-mail: jfc@unizar.es

M. F. Rañada
e-mail: mfran@unizar.es

M. Santander
Departamento de Física Teórica and IMUVa, Facultad de Ciencias,
Universidad de Valladolid, 47011 Valladolid, Spain
e-mail: mariano.santander@uva.es

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_7

7.1 Introduction

Many attempts have been done during the last recent years to clarify and to establish a common geometric approach to both Classical and Quantum Mechanics and the transition from Classical to Quantum Mechanics (see e.g. [1–3]). Symplectic geometry has been shown to be the common framework for dealing with both types of systems [4].

On one hand, the geometric framework for the description of classical mechanical systems is the theory of Hamiltonian dynamical systems [5, 6]. A symplectic structure ω on a differentiable manifold M, or more generally a Poisson structure, is the basic concept. It is then possible to define an associated Poisson bracket endowing the set of functions on M with a real Lie algebra structure. The dynamics is given by the Hamiltonian vector field X_H defined by the Hamiltonian $H \in C^\infty(M)$ by means of $i(X_H)\omega = dH$. The system of differential equations determining the integral curves of X_H in Darboux coordinates are Hamilton equations. A particularly interesting case is when the manifold is the cotangent bundle of the configuration space Q, $M = T^*Q$, endowed with its natural exact symplectic structure. Then, the states in Classical Mechanics are the points of M, while the observables are the functions $F \in C^\infty(M)$. The measure of an observable F in a state $x \in M$ is given by the evaluation map, the result being $F(x)$.

On the other side, the mathematical model for Quantum Theories is different. In Quantum Mechanics in Schrödinger picture, (pure) states are (rays rather than) vectors ψ of a separable complex Hilbert space $(\mathcal{H}, \langle\cdot,\cdot\rangle)$, while observables are the elements of $\mathcal{A}(\mathcal{H})$, the set of selfadjoint operators in $\mathcal{H}$. The results of the measure of the observable A in the pure state ψ may be any eigenvalue of A but with probabilities such that the mean value is

$$e_A(\psi) = \frac{\langle\psi, A\psi\rangle}{\langle\psi, \psi\rangle}. \tag{7.1}$$

Finally, the dynamics is given by Schrödinger equation.

Both Classical and Quantum Mechanics can be seen as particular instances of a more general theory. Actually, the framework unifying both approaches is the theory of Hamiltonian dynamical systems. Then in Sect. 7.2 we recall the basic geometric ingredients of geometric approach to Classical Mechanics and in Sect. 7.3 we study the particular case of mechanical type systems, while in Sect. 7.4 we recall the formulation of Quantum Mechanics from the perspective of Hamiltonian dynamical systems theory. This enables us to better understand the relationship, analysed in Sect. 7.5, between Classical and Quantum mechanics, particularly in cases where the configuration space is not $\mathbb{R}^n$. As two instances the simple examples of position-dependent mass systems and motions on curves are presented in Sects. 7.6 and 7.7 in the classical approach and Sects. 7.8 and 7.9 in the quantum one. The last Sections are devoted to the important case of motions on constant curvature surfaces and a summary of conclusions and output.

7.2 Hamiltonian Dynamical Systems

A symplectic manifold is a pair (M, ω) where M is a differentiable manifold and ω is a symplectic form, i.e. a non-degenerate closed 2-form in M, $\omega \in Z^2(M)$, $d\omega = 0$ [5, 6]. Non-degeneracy of ω means that for every point $u \in M$ the map $\widehat{\omega}_u : T_uM \to T_u^*M$, given by $\langle \widehat{\omega}_u(v), v' \rangle = \omega_u(v, v')$, $\forall v, v' \in T_uM$, is a bijection. This implies that the dimension of M is even, $\dim M = 2n$.

The map $\widehat{\omega} : TM \to T^*M$ is a base-preserving fibred map, and therefore it induces a $C^\infty(M)$-linear map between the $C^\infty(M)$-modules of sections of both bundles which, with a slight abuse of notation, we also write $\widehat{\omega} : \mathfrak{X}(M) \to \bigwedge^1(M)$. The vector fields corresponding to closed 1-forms are called locally-Hamiltonian vector fields and those corresponding to exact 1-forms are said to be Hamiltonian vector fields, i.e. $\widehat{\omega}(\mathfrak{X}_{\mathrm{H}}(M, \omega)) = B^1(M)$ and $\widehat{\omega}(\mathfrak{X}_{\mathrm{LH}}(M, \omega)) = Z^1(M)$. So, if $H \in C^\infty(M)$, the Hamiltonian vector field X_H is defined as the vector field such that

$$i(X_H)\omega = dH. \tag{7.2}$$

We say that (M, ω, H) is a Hamiltonian system when (M, ω) is a symplectic manifold and $H \in C^\infty(M)$: the dynamical vector field is X_H. Cartan identity, $\mathcal{L}_X = i(X) \circ d + d \circ i(X)$, shows that $X \in \mathfrak{X}_{\mathrm{LH}}(M, \omega)$ if and only if $\mathcal{L}_X \omega = 0$. An example is that of the cotangent bundle $\pi_Q : T^*Q \to Q$ of a differentiable manifold Q. There is a canonical 1-form θ_0 on T^*Q, that in a local chart of T^*Q, $(\pi_Q^{-1}(U), \phi)$, where $\phi = (q^1, \ldots, q^n; p_1, \ldots, p_n)$, induced by a chart (U, φ) of Q, $\varphi = (q^1, \ldots, q^n)$, has the local expression $\theta_0 = \sum_{i=1}^n p_i\, dq^i$, and then the 2-form $\omega_0 = -d\theta_0$ with local expression $\sum_{i=1}^n dq^i \wedge dp_i$ is a symplectic form.

This is the local prototype of a symplectic manifold, because Darboux proved that $d\omega = 0$ and regularity of ω imply that around each point $u \in M$ there is a local chart (U, ϕ) such that if $\phi = (q^1, \ldots, q^n; p_1, \ldots, p_n)$, then $\omega|_U = \sum_{i=1}^n dq^i \wedge dp_i$. Such coordinates are said to be Darboux coordinates and the local expression of X_H is given by

$$X_H = \sum_{i=1}^{n} \left(\frac{\partial H}{\partial p_i} \frac{\partial}{\partial q^i} - \frac{\partial H}{\partial q^i} \frac{\partial}{\partial p_i} \right), \tag{7.3}$$

and therefore, the local equations determining its integral curves are similar to Hamilton equations.

The *Poisson bracket* of two functions $f, g \in C^\infty(M)$ is defined as the function $\{f, g\}$ given by:

$$\{f, g\} = \omega(X_f, X_g) = df(X_g) = -dg(X_f) = X_g f = -X_f g, \tag{7.4}$$

which in Darboux coordinates for ω reduces to the usual expression. The map $\{\cdot, \cdot\} : C^\infty(M) \times C^\infty(M) \to C^\infty(M)$ is skew-symmetric and $\mathbb{R}$-bilineal. Closeness of ω implies that $\{\cdot, \cdot\}$ satisfies the Jacobi identity, therefore $\{\cdot, \cdot\}$ endows $C^\infty(M)$ with a real Lie algebra structure. Moreover, if X, Y are locally Hamiltonian vector fields,

then $[X, Y]$ is a Hamiltonian vector field, its Hamiltonian being $\omega(Y, X)$. In fact, it is a consequence of the relation $i(X)\mathcal{L}_Y\alpha - \mathcal{L}_Y i(X)\alpha = i([X, Y])\alpha$, which is valid for any form α. Then,

$$i([X, Y])\omega = i(X)\mathcal{L}_Y\omega - \mathcal{L}_Y i(X)\omega = -\mathcal{L}_Y i(X)\omega = -i(Y)d[i(X)\omega] - d[i(Y)i(X)\omega] = -d[\omega(X, Y)].$$

In particular, when $X = X_f$ and $Y = X_g$ in the previous relation, $d\{f, g\} = -i([X_f, X_g])\omega$, i.e. $[X_f, X_g] = X_{\{g,f\}}$. This shows that the set of Hamiltonian vector fields, to be denoted $\mathfrak{X}_{\mathrm{H}}(M, \omega)$, is an ideal of the Lie algebra of locally-Hamiltonian vector fields $\mathfrak{X}_{\mathrm{LH}}(M, \omega)$ and that

$$0 \longrightarrow \mathbb{R} \longrightarrow C^\infty(M) \xrightarrow{\sigma} \mathfrak{X}_{\mathrm{H}}(M, \omega) \longrightarrow 0,$$

with $\sigma = -\widehat{\omega}^{-1} \circ d$, is an exact sequence of Lie algebras.

An action Φ of a Lie group G with Lie algebra $\mathfrak{g}$ on M defines a set of fundamental vector fields $X_a \in \mathfrak{X}(M), a \in \mathfrak{g}$, by $X_a(m) = \Phi_{m*e}(-a)$ and the map $X : \mathfrak{g} \to \mathfrak{X}(M)$, $a \in \mathfrak{g} \to X_a$ is a Lie algebra homomorphism, i.e. $[X_a, X_b] = X_{[a,b]}$. If the action of G is strongly symplectic, $X(\mathfrak{g}) \subset \mathfrak{X}_{\mathrm{H}}(M, \omega)$, then X is a Lie algebra homomorphism $X : \mathfrak{g} \to \mathfrak{X}_{\mathrm{H}}(M, \omega)$, and then there exists a linear map $f : \mathfrak{g} \to C^\infty(M)$, called comomentum map, making commutative the following diagram:

$$\begin{array}{ccccccccc} & & & & & & \mathfrak{g} & & \\ & & & & & \overset{f}{\swarrow} & \downarrow X & & \\ 0 & \longrightarrow & \mathbb{R} & \longrightarrow & C^\infty(M) & \xrightarrow{\sigma} & \mathfrak{X}_{\mathrm{H}}(M, \omega) & \longrightarrow & 0 \end{array}$$

The corresponding momentum map introduced by Souriau, is the map $P : M \to \mathfrak{g}^*$, defined by

$$\langle P(m), a\rangle = f_a(m), \qquad \forall m \in M, a \in \mathfrak{g}. \tag{7.5}$$

It is not uniquely defined but two possible comomentum maps differ by a linear map $r : \mathfrak{g} \to \mathbb{R}, f'_a(m) = f_a(m) + r(a)$. In case of exact symplectic actions on exact symplectic manifolds $(M, \omega = -d\theta)$, namely, $g^*\theta = \theta$, $\forall g \in G$, the fundamental vector fields X_a are Hamiltonian and a comomentum map can be defined as $f_a = -i(X_a)\theta$. This is the case of an action of a Lie group G on a cotangent bundle T^*Q lifted from an action of G on its base manifold. Recall that if $X = \sum_{i=1}^n \xi^i(q)\partial/\partial q^i \in \mathfrak{X}(Q)$, its cotangent lift $\widetilde{X} \in \mathfrak{X}(T^*Q)$ ($\widetilde{X}$ projectable on X and satisfying $\mathcal{L}_{\widetilde{X}}\theta_0 = 0$, with θ_0 the Liouville 1-form, $\theta = \sum_{i=1}^n p_i\, dq^i$), is

$$\widetilde{X} = \sum_{i=1}^n \xi^i \frac{\partial}{\partial q^i} - \sum_{i,j=1}^n p_i \frac{\partial \xi^i}{\partial q^j}\frac{\partial}{\partial p_j}. \tag{7.6}$$

As an instance, if the configuration space is $Q = \mathbb{R}^3$ we can consider vector fields generating translations on $Q = \mathbb{R}^3$, and their corresponding lift in $T^*\mathbb{R}^3$, the fundamental vector fields in $\mathbb{R}^3$ being $X_a = -\sum_{i=1}^n a^i\, \partial/\partial q^i$, with canonical lifts $\widetilde{X}_a$ a $T^*\mathbb{R}^3$, given by $\widetilde{X}_a = -\sum_{i=1}^n a^i\, \partial/\partial q^i$. The functions $f_a \in C^\infty(T^*\mathbb{R}^3)$ are defined by $f_a(q,p) = -[i(\widetilde{X}_a)\theta](q,p) = \sum_{i=1}^n a^i p_i$. Using $f_a(q,p) = \langle \mathbf{P}(q,p), a\rangle$ and identifying $\mathbb{R}^3$, as Lie algebra of translations, with its dual, we obtain $\mathbf{P}(q,p) = \mathbf{p}$.

If the usual action of $SO(3,\mathbb{R})$ on $\mathbb{R}^3$ and the induced action on $T^*\mathbb{R}^3$ are considered, the fundamental vector fields in $\mathbb{R}^3$ are $X_i = -\sum_{j,k=1}^n \epsilon_{ijk}\, q^j\, \partial/\partial q^k$, with canonical lifts

$$\widetilde{X}_i = -\sum_{j,k=1}^{n} \epsilon_{ijk} \left(q^j \frac{\partial}{\partial q^k} - p_j \frac{\partial}{\partial p_k} \right),$$

and consequently a comomentum map is $f_{\mathbf{n}}(q,p) = \sum_{i,j,k=1}^n n_i\, \epsilon_{ijk}\, q^j\, p_k = \mathbf{n} \cdot (\mathbf{q} \times \mathbf{p})$. Using the identification of $\mathbb{R}^3$ with its dual space we see that $\mathbf{P}(q,p) = \mathbf{q} \times \mathbf{p}$, i.e. the associated momentum is the angular momentum.

7.3 Dynamical Systems of Mechanical Type

A particularly interesting example of symplectic structure is the one defined in a tangent bundle $\tau_Q : TQ \to Q$ by a regular Lagrangian $L \in C^\infty(TQ)$. Two important geometric ingredients of the tangent bundle $\tau_Q : TQ \to Q$ are the Liouville vector field Δ, that is the generator of dilations along the fibres,

$$\Delta f(v) = \frac{d}{dt} f(e^t v)|_{t=0}, \qquad \forall v \in TQ,\, f \in C^\infty(TQ). \tag{7.7}$$

and the vertical endomorphism S (see e.g. [1, 7, 8]). Given the differentiable function L on TQ, we can construct a semibasic 1-form $\theta_L \in \bigwedge^1(TQ)$, an exact 2-form $\omega_L \in \bigwedge^2(TQ)$ and an energy function by

$$\theta_L = S^*(dL) = dL \circ S\,, \quad \omega_L = -d\theta_L\,, \quad E_L = \Delta(L) - L\,, \tag{7.8}$$

and when the 2-form $\omega_L = -d\theta_L$ is of maximal rank, and therefore symplectic, the Lagrangian L is said to be regular. The Lagrangian dynamics is given by the uniquely determined vector field Γ_L solution of

$$i(\Gamma_L)\omega_L = dE_L. \tag{7.9}$$

Γ_L satisfies the second-order property $S(\Gamma_L) = \Delta$, and the curves on Q that are a projection of the integrals curves of Γ_L in TQ satisfy the second-order Euler–Lagrange equations [7, 8].

We are now interested in regular natural Lagrangian systems given by a non-degenerate symmetric (0, 2)-tensor field g on the configuration space Q and a function V on Q: $L \in C^\infty(TQ)$ is given by [9]

$$L_{g,V}(v) = \frac{1}{2}(\tau_Q^* g)(v, v) + \tau^* V. \tag{7.10}$$

Nondegeneracy of g means that the map $\widehat{g} : TQ \to T^*Q$ defined by $\langle \widehat{g}(v), w\rangle = g(v, w)$, where $v, w \in T_xQ$, is regular. Note that $\widehat{g}$ is a fibred map over the identity on Q and induces an isomorphism between the corresponding linear spaces of sections $\widehat{g} : \mathfrak{X}(Q) \to \bigwedge^1(Q)$: $\langle \widehat{g}(X), Y\rangle = g(X, Y)$. If $f \in C^\infty(Q)$ the vector field corresponding to the exact 1-form df is denoted $\mathrm{grad} f$, i.e. $\widehat{g}(\mathrm{grad} f) = df$.

The case $V = 0$ in (7.10) corresponds to free motion on the (pseudo-)Riemann manifold (Q, g), the Lagrangian then being given by the kinetic energy defined by the metric g:

$$L_{g,0}(v) = T_g(v) = \frac{1}{2}(\tau_Q^* g)(v, v), \qquad v \in TQ, \tag{7.11}$$

which can be rewritten as the function on TQ

$$T_g = \frac{1}{2}\, g(T\tau_Q \circ D, T\tau_Q \circ D), \tag{7.12}$$

with D being any second order differential equation vector field, i.e. a vector field on TQ, and therefore $\tau_{TQ} \circ D = \mathrm{id}_{TQ}$, such that also $T\tau_Q \circ D = \mathrm{id}_{TQ}$.

If $(U, q^1, \ldots, q^n)$ is a local chart on Q, we can consider the coordinate basis of $\mathfrak{X}(U)$, usually denoted $\{\partial/\partial q^j \mid j = 1, \ldots, n\}$, and its dual basis for $\bigwedge^1(U)$, $\{dq^j \mid j = 1, \ldots, n\}$. A vector and a covector in a point $q \in U$ are $v = v^j\,(\partial/\partial q^j)_q$ and $\zeta = p_j\,(dq^j)_q$, with $v^j = \langle dq^j, v\rangle$ and $p_j = \langle \zeta, \partial/\partial q^j\rangle$. These are Darboux coordinates and the local expressions for g, T_g and $\mathrm{grad} f$) are:

$$g = \sum_{i,j=1}^{n} g_{ij}(q)\, dq^i \otimes dq^j, \qquad T_g(v) = \frac{1}{2}\sum_{i,j=1}^{n} g_{ij}(\tau_Q(v))\, v^i v^j,$$

$$(\mathrm{grad} f)^i = \sum_{j=1}^{n} g^{ij}\frac{\partial f}{\partial q^j}, \tag{7.13}$$

with $\sum_{k=1}^n g^{ik}(q)\, g_{kj}(q) = \delta^i_j$. The dynamics is then given by a vector field $\Gamma_{L_{g,V}}$ solution of

$$i(\Gamma_{L_{g,V}})\omega_{L_{g,V}} = dE_{L_{g,V}}. \tag{7.14}$$

where the energy $E_{L_{g,V}}$ of the Lagrangian system is defined by $E_{L_{g,V}} = \Delta L_{g,V} - L_{g,V}$. As $\Delta(T_g) = 2\,T_g$ and $\Delta(V) = 0$, the total energy is $E_{L_{g,V}} = T_g + V$. The Cartan 1-form, $\theta_{L_{g,V}} = dL_{g,V} \circ S = \theta_{T_g}$ (see e.g. [7, 8]), gives us an exact 2-form $\omega_{L_{g,V}} = \omega_{T_g} = -d\theta_{T_g}$, which is non-degenerate when g is regular and then $(TQ, \omega_{L_{g,V}}, E_{L_{g,V}})$

is a Hamiltonian dynamical system. Their coordinate expressions are:

$$\theta_{L_{g,V}}(q,v) = \sum_{i,j=1}^{n} g_{ij}(q)\, v^j\, dq^i,$$

$$\omega_{L_{g,V}} = \sum_{i,j=1}^{n} g_{ij}\, dq^i \wedge dv^j + \frac{1}{2}\sum_{i,j,k=1}^{n}\left(\frac{\partial g_{ij}}{\partial q^k}v^j - \frac{\partial g_{kj}}{\partial q^i}v^j\right) dq^i \wedge dq^k. \quad (7.15)$$

To be remarked that $\omega_{L_{g,V}}$ only depends on T_g and not on V, and we can use ω_{T_g} instead of $\omega_{L_{g,V}}$.

Moreover, it has been proved in [9] that if $X \in \mathfrak{X}(Q)$ and $X^c \in \mathfrak{X}(TQ)$ is its complete lift [7, 8],

$$X^c T_g = T_{\mathcal{L}_X g}, \quad (7.16)$$

and this property can be used to prove that the lifts of the flow of X are exact symplectomorphisms if and only if $\mathcal{L}_X g = 0$, i.e. X is a Killing vector field. Actually, $\mathcal{L}_{X^c}\theta_{L_{g,V}} = \mathcal{L}_{X^c}\theta_{T_g} = \theta_{X^c(T_g)} = \theta_{T_{\mathcal{L}_X g}}$, and consequently, if X is a Killing vector field, $\mathcal{L}_{X^c}\omega_{L_{g,V}} = 0$ and $i(X^c)\omega_L = d\,(i(X^c)\theta_L$. Moreover, $X^c(T_g) = 0$. In other words, the complete lift of a Killing vector field for g is a symmetry of the free Lagrangian T_g and provides a constant for this free motion. Recall also that Killing vector fields close under commutators on a finite-dimensional Lie algebra.

The relation of Lagrangian and Hamiltonian formalism is established by means of the Legendre transformation $\mathcal{F}L : TQ \to T^*Q$, which is a diffeomorphism, because the $(0,2)$-symmetric tensor g is assumed to be non-degenerate: If $v \in T_qQ$, then $\alpha = \mathcal{F}L(v) \in T_q^*Q$ is such that $\langle \alpha, w\rangle = g(v,w), \forall w \in T_qQ$. In the above mentioned local coordinates

$$p_i = \frac{\partial T_g}{\partial v^i} = \sum_{k=1}^{n} g_{ik}(q)\, v^k \iff v^i = \sum_{j=1}^{n} g^{ij}(q)\, p_j. \quad (7.17)$$

The remarkable fact is that $\theta_L = \mathcal{F}L^*\theta_0$, and then a comparison of (7.2) with (7.8) shows that $\omega_{T_g} = \mathcal{F}L^*\omega_0$, and that $\mathcal{F}L_*(\Gamma_{T_g}) = X_{H_g}$ when the Hamiltonian H_g for the free motion is the function corresponding to the kinetic energy in terms of momenta, i.e. $H_g = E_g \circ \mathcal{F}L^{-1}$:

$$H_g = \frac{1}{2}g(\widehat{g}^{-1}(p), \widehat{g}^{-1}(p)) = \frac{1}{2}\sum_{i,j=1}^{n} g^{ij}\, p_i\, p_j. \quad (7.18)$$

If we consider the exact symplectic action of a Lie group G on the bundle T^*Q defined by lifting an action of G on the base Q, if $X_a = \sum_{i=1}^n \xi_a^i(q)\,\partial/\partial q^i$ is the infinitesimal generator of $a \in \mathfrak{g}$ in the action on Q its lifting is given in the induced coordinate system by the expression (7.6), and when $\widetilde{X}_a$ is Hamiltonian, as $\theta_0 = \sum_{i=1}^n p_i\, dq^i$ we have that $f_a(q,p) = -\sum_{i=1}^n p_i\, \xi_a^i(q)$.

In the particular case of a natural Lagrangian system as the complete lift $X^c \in \mathfrak{X}(TQ)$ of a Killing vector field $X \in \mathfrak{X}(Q)$ is a Hamiltonian vector field, we have an exact action of the Lie algebra of Killing vector fields on TQ and the momentum map $P_{\mathrm{L}} : TQ \to \mathfrak{kill}^*$ is defined by

$$\langle P_{\mathrm{L}}(x, v), a\rangle = f_a(x, v) = -\theta_{T_g}(X_a^c) = -\sum_{i,j=1}^{n} g_{ij} v^j \xi_a^i, \qquad (x, v) \in TQ,\ a \in \mathfrak{kill}. \tag{7.19}$$

On the other side, there is an alternative way to lift to T^*Q Killing vector fields X_a on a Riemann manifold (Q, g). Define $\bar{X}_a = \mathcal{F}L_*(X_a^c)$ and then these vector fields in T^*Q span a Lie algebra isomorphic to the Killing algebra, and are Hamiltonian with respect to ω_0, because $i(\bar{X}_a)\theta_0 = i(\mathcal{F}L_*(X_a^c))\theta_0 = (i(X_a^c)\theta_L) \circ \mathcal{F}L^{-1}$, and the momentum map P_{H} in the corresponding Hamiltonian formalism, $P_{\mathrm{H}} : T^*Q \to \mathfrak{kill}^*$ is given by

$$\langle P_{\mathrm{H}}(x, p), a\rangle = \bar{f}_a(x, p) = -\theta_0(\bar{X}_a), \qquad (x, p) \in T^*Q, a \in \mathfrak{kill}, \tag{7.20}$$

with $\bar{f}_a = f_a \circ \mathcal{F}L^{-1}$, i.e. $P_{\mathrm{H}} = P_{\mathrm{L}} \circ \mathcal{F}L^{-1}$.

7.4 Geometric Approach to Quantum Mechanics

The Schrödinger picture of Quantum mechanics admits a geometric interpretation similar to that of classical mechanics [1, 4]. A separable complex Hilbert space $(\mathcal{H}, \langle\cdot,\cdot\rangle)$ can be considered as a real linear space, to be then denoted $\mathcal{H}_{\mathbb{R}}$. The norm in $\mathcal{H}$ defines a norm in $\mathcal{H}_{\mathbb{R}}$, where $\|\psi\|_{\mathbb{R}} = \|\psi\|_{\mathbb{C}}$. The linear real space $\mathcal{H}_{\mathbb{R}}$ is endowed with a natural symplectic structure as follows:

$$\omega(\psi_1, \psi_2) = 2\,\mathrm{Im}\langle\psi_1, \psi_2\rangle. \tag{7.21}$$

The Hilbert $\mathcal{H}_{\mathbb{R}}$ can be considered as a real manifold modeled by a Banach space admitting a global chart. The tangent space $T_\phi\mathcal{H}_{\mathbb{R}}$ at any point $\phi \in \mathcal{H}_{\mathbb{R}}$ can be identified with $\mathcal{H}_{\mathbb{R}}$ itself; the isomorphism associates $\psi \in \mathcal{H}_{\mathbb{R}}$ with the vector $\dot{\psi} \in T_\phi\mathcal{H}_{\mathbb{R}}$ given by:

$$\dot{\psi} f(\phi) := \left(\frac{d}{dt} f(\phi + t\psi)\right)_{|t=0}, \qquad \forall f \in C^\infty(\mathcal{H}_{\mathbb{R}})\,. \tag{7.22}$$

The real manifold can be endowed with a symplectic 2-form ω:

$$\omega_\phi(\dot{\psi}, \dot{\psi}') = 2\,\mathrm{Im}\,\langle\psi, \psi'\rangle. \tag{7.23}$$

One can see that the constant symplectic structure ω in $\mathcal{H}_{\mathbb{R}}$, considered as a Banach manifold, is exact, i.e., there exists a 1-form $\theta \in \bigwedge^1(\mathcal{H}_{\mathbb{R}})$ such that $\omega = -d\theta$. For instance, the one defined by $\theta(\psi_1)[\dot{\psi}_2] = -\mathrm{Im}\langle\psi_1, \psi_2\rangle$. This shows that the geometric framework for usual Schrödinger picture is that of symplectic mechanics, as in the classical case.

In order to avoid topological sutilities we restrict ourselves to finite-dimensional Hilbert spaces. A continuous vector field in $\mathcal{H}_{\mathbb{R}}$ is a continuous map $X : \mathcal{H}_{\mathbb{R}} \to \mathcal{H}_{\mathbb{R}}$. For instance for each $\phi \in \mathcal{H}$, the constant vector field X_ϕ defined by $X_\phi(\psi) = \dot{\phi}$. It is the generator of the one-parameter subgroup of transformations of $\mathcal{H}_{\mathbb{R}}$ given by $\Phi(t, \psi) = \psi + t\,\phi$. As another particular example of vector field, consider the vector field X_A defined by the $\mathbb{C}$-linear map $A : \mathcal{H} \to \mathcal{H}$, and in particular when A is skew-selfadjoint, as follows. With the natural identification natural of $T\mathcal{H}_{\mathbb{R}} \approx \mathcal{H}_{\mathbb{R}} \times \mathcal{H}_{\mathbb{R}}$, X_A is given by $X_A : \phi \mapsto (\phi, A\phi) \in \mathcal{H}_{\mathbb{R}} \times \mathcal{H}_{\mathbb{R}}$. When $A = I$ the vector field X_I is the Liouville generator of dilations along the fibres, $\Delta = X_I$, usually denoted Δ, given by $\Delta(\phi) = (\phi, \phi)$. The remarkable fact, to be proved next, is that when A is skew-selfadjoint, the vector field $X_{-\mathrm{i}A}$ is Hamiltonian.

Given a selfadjoint operator A in $\mathcal{H}$ we can define a real function in $\mathcal{H}_{\mathbb{R}}$ by $a(\phi) = \langle\phi, A\phi\rangle$, i.e. $a = \langle\Delta, X_A\rangle$. Then, $da_\phi(\psi) = \frac{d}{dt}a(\phi + t\psi)_{t=0} = \frac{d}{dt}\,[\langle\phi + t\psi, A(\phi + t\psi)\rangle]_{|t=0} = 2\,\mathrm{Re}\,\langle\psi, A\phi\rangle = 2\,\mathrm{Im}\,\langle -\mathrm{i}A\phi, \psi\rangle = \omega(-\mathrm{i}A\phi, \psi)$. If we recall that the Hamiltonian vector field defined by the function a is such that for each $\psi \in T_\phi\mathcal{H} = \mathcal{H}$, $da_\phi(\psi) = \omega(X_a(\phi), \psi)$, we see that

$$X_a(\phi) = -\mathrm{i}\,A\phi\,. \tag{7.24}$$

Therefore if A is the Hamiltonian H of a quantum system, the Schrödinger equation describing time-evolution plays the rôle of 'Hamilton equations' for the Hamiltonian dynamical system $(\mathcal{H}, \omega, h)$, where $h(\phi) = \langle\phi, H\phi\rangle$, because the integral curves of X_h satisfy

$$\dot{\phi} = X_h(\phi) = -\mathrm{i}\,H\phi\,. \tag{7.25}$$

The real functions $a(\phi) = \langle\phi, A\phi\rangle$ and $b(\phi) = \langle\phi, B\phi\rangle$ corresponding to two selfadjoint operators A and B satisfy [10]

$$\{a, b\}(\phi) = -\mathrm{i}\,\langle\phi, [A, B]\phi\rangle\,, \tag{7.26}$$

because $\{a, b\}(\phi) = [\omega(X_a, X_b)](\phi) = \omega_\phi(X_a(\phi), X_b(\phi)) = 2\,\mathrm{Im}\,\langle A\phi, B\phi\rangle$, and taking into account that

$$2\,\mathrm{Im}\,\langle A\phi, B\phi\rangle = -\mathrm{i}\,[\langle A\phi, B\phi\rangle - \langle B\phi, A\phi\rangle] = -\mathrm{i}\,[\langle\phi, AB\phi\rangle - \langle\phi, BA\phi\rangle]\,,$$

we find the above result. So, on the integral curves of the vector field X_h defined by a Hamiltonian H,

$$\dot{a}(\phi) = \{a, h\}(\phi) = -\mathrm{i}\,\langle\phi, [A, H]\phi\rangle\,, \tag{7.27}$$

what is usually known as Ehrenfest theorem:

$$\frac{d}{dt}\langle\phi, A\phi\rangle = -\mathrm{i}\,\langle\phi, [A, H]\phi\rangle\,.$$

There is another relevant symmetric (0, 2) tensor field which is given by the real part of the inner product. It endows $\mathcal{H}_{\mathbb{R}}$ with a Riemann structure and tnere is also a complex structure J in $\mathcal{H}_{\mathbb{R}}$, the $\mathbb{R}$ linear map corresponding to multiply by i, such that

$$g(v_1, v_2) = -\omega(Jv_1, v_2), \quad \omega(v_1, v_2) = g(Jv_1, v_2),$$
$$g(Jv_1, Jv_2) = g(v_1, v_2), \omega(Jv_1, Jv_2) = \omega(v_1, v_2).$$

The triplet (g, J, ω) defines a Kähler structure in $\mathcal{H}_{\mathbb{R}}$ and the symmetry group of the theory must be the unitary group $U(\mathcal{H})$ whose elements preserve the inner product, or in an alternative (but equivalent in the finite-dimensional case) way, by the intersection of the orthogonal group $O(2n, \mathbb{R})$ and the symplectic group $Sp(2n, \mathbb{R})$.

On the other hand, as the relevant concept for measurements is the expectation value of observables, we should consider as indistinguishable two vectors ψ_1 and ψ_2 such that $e_A(\psi_2) = e_A(\psi_1)$, for each selfadjoint operator A. This is only possible when ψ_2 is proportional to ψ_1. In fact it suffices to take as observable A the orthogonal projection on ψ_1. Therefore we must consider rays rather than vectors the elements describing the quantum states and consequently the space of states is not $\mathbb{C}^n$, in the finite-dimensional case, but the projective space $\mathbb{CP}^{n-1}$. However it is possible to define a related Kähler structure on $\mathbb{CP}^{n-1}$ and many similar geometric techniques can be used in this case.

7.5 How to Find a Quantum Model for a Classical One?

In general the problem of 'quantisation' of a system is, given a classical Hamiltonian system (M, ω, H), to find a Hilbert space $\mathcal{H}$ and to choose the selfadjoint operator $\widehat{F}$ corresponding to the relevant observables F. In the simplest case of an Euclidean configuration space, the prescription is that $\mathcal{H}$ is the space of square integrable functions with respect to the Lebesgue measure, positions $\widehat{x}_i$ have associated multiplication by x_i operators and the momentum operators are the differential operators $\widehat{p}_k = -\mathrm{i}\,\partial/\partial x_k$. There will be some ordering ambiguities for other observables because functions of x_i commute with those of p_k, but $\widehat{x}_i$ does not commute with $\widehat{p}_k$, because we have $[\widehat{x}_i, \widehat{p}_j] = \mathrm{i}\,\delta_{ik}$, as corresponding to $\{x_i, p_k\} = \delta_{ik}$.

Many textbooks warn that this canonical quantisation rule is only valid using Euclidean coordinates. This is very restrictive, because, What happens in other coordinates and, even worse, when there are no global preferred coordinates (for instance Q is compact)? and What about position-dependent mass for which mass operator does not commute with momentum operators?

Generalising previous procedure for a more general case of a Hamiltonian dynamical system, Dirac assertion is that *Quantisation is to be understood as a map* $\zeta : C^\infty(M) \to \mathcal{A}(\mathcal{H})$ *such that* $-i\zeta(\{F, G\}) = [\zeta(F), \zeta(G)]$, to be compared with (7.26).

In order to clarify the situation we start by pointing out that in classical mechanics, if the configuration space is an Euclidean space $\mathbb{R}^n$, p_i denotes many different and inequivalent objects. So, p_i denotes the i-th coordinate of a covector in a point of the configuration space, but also p_i is a real function in $T^*\mathbb{R}^n$ defined as $p_i(\alpha) = \alpha(\partial/\partial x_i)$. Finally, the real function p_i is the infinitesimal generator of translations along the i-th coordinate axis, which are canonical transformations for $(T^*\mathbb{R}^n, \omega_0)$.

In a more general case, $Q \neq T^*\mathbb{R}^n$, there is not a global chart, the momentum coordinates are local and depend on the choice of base manifold coordinates, and translations are not defined. Recall however that translations and rotations are isometries of the Euclidean space.

For natural Lagrangians defined on TQ, with Q an arbitrary Riemann manifold, we can consider the isometries of the Riemann metric, whose above mentioned lifts are Hamiltonian vector fields and in this way we define a strongly symplectic action on T^*Q of the group of isometries of the Riemann manifold.

We are then able to define an associated momentum. The components P_a of this map are the objects to be quantised instead of the p_i which is not an intrinsic but a coordinate dependent ingredient. This allows us to quantise functions of the momentum map by associating the function P_a with $\widehat{P}_a = -\mathrm{i}\, X_a$ acting on an appropriate Hilbert space. Consequently, we can quantise functions of the momentum map. We next consider some simple models to see how this works.

7.6 Position Dependent Mass Systems

Consider a 1-dimensional system described in terms of a coordinate x by a Lagrangian [10]

$$L = \frac{1}{2}\, m(x)\dot{x}^2 - V(x)\,, \quad x \in \mathbb{R}\,, \quad m(x) > 0, \tag{7.28}$$

leading to the nonlinear differential equation $m(x)\,\ddot{x} + \frac{1}{2}\, m'(x)\,\dot{x}^2 = 0$. The associated Hamiltonian H is

$$H(x, p) = \frac{1}{2}\,\frac{1}{m(x)}\, p^2 + V(x). \tag{7.29}$$

There is an important problem with the construction of the quantum version $\widehat{H}$ of H, from the classical system to the quantum one, because if the mass m is a function of the spatial coordinate, $m = m(x)$, then the quantum version of the mass no longer commutes with the momentum. Different forms of presenting the kinetic term in the Hamiltonian H, as for example

$$T = \frac{1}{4}\left[\frac{1}{m(x)}\,p^2 + p^2\,\frac{1}{m(x)}\right], \quad T = \frac{1}{2}\left[\frac{1}{\sqrt{m(x)}}\,p^2\,\frac{1}{\sqrt{m(x)}}\right],$$
$$T = \frac{1}{2}\left[p\,\frac{1}{m(x)}\,p\right],$$

are classically equivalent but they lead to different and nonequivalent Schrödinger equations [11–13].

This problem is important mainly because there are a certain number of important areas, mainly related with problems on condensed-matter physics (electronic properties of semiconductors, liquid crystals, quantum dots, etc.), in which the behaviour of the system depends of an effective mass that is position-dependent [14, 15]. Furthermore, from a more conceptual viewpoint, the ordering of factors in the transition from a commutative to a noncommutative formalism is an old question that remains as an important open problem in the theory of quantisation.

On the other side, the free motion along a simple regular curve C looks like a position–dependent mass system. If C is given in parametric form by $\mathbf{x} : I \to \mathbb{R}^n$, $u \mapsto \mathbf{x}(u)$, its arc-length function $s(u)$ is an intrinsic parameter given by

$$\frac{ds}{du} = \sqrt{\frac{d\mathbf{x}}{du}\cdot\frac{d\mathbf{x}}{du}} = f(u) > 0, \qquad s(u) = \int^u \sqrt{\dot{\mathbf{x}}(\zeta)\cdot\dot{\mathbf{x}}(\zeta)}\,d\zeta. \tag{7.30}$$

The geodesics of this metric coincide, up to reparametrisation, with the curves solution of the Euler–Lagrange equation of the Lagrangian $L_0(s, \dot{s}) = \frac{1}{2}\,m_0\,\dot{s}^2$ [16], that in terms of coordinate u becomes

$$L_0(u, v_u) = \frac{1}{2}\,m_0 f(u)\,v_u^2, \tag{7.31}$$

where m_0 is a constant with mass dimension, i.e. if $f'(u) = df/du$,

$$\frac{d}{dt}(f(u)\dot{u}) = \frac{1}{2}f'(u)\,\dot{u}^2 \Longrightarrow f(u)\,\ddot{u} + \frac{1}{2}f'(u)\,\dot{u}^2 = 0. \tag{7.32}$$

7.7 Classical Motion on a Cycloid: A Case Study

As an illustrative example, consider the motion of a particle of mass m_0 moving on a gravitational field along a cycloid inverted in such a way that the origin is sited in the lowest point [17, 18], namely:

$$\mathbf{x}(\vartheta) = (R(\vartheta + \pi + \sin\vartheta), R(1 - \cos\vartheta)) = \left(R(\vartheta + \pi + \sin\vartheta), 2R\,\sin^2\frac{\vartheta}{2}\right),$$
$$\vartheta \in (-\pi, \pi). \tag{7.33}$$

Consequently, $\dot{\mathbf{x}}(\vartheta) = (R(1+\cos\vartheta), R\sin\vartheta)$, and then,

$$\|\dot{\mathbf{x}}\|^2 = R^2(1+\cos^2\vartheta + 2\cos\vartheta + \sin^2\vartheta) = 2R^2(1+\cos\vartheta) = 4R^2\cos^2\frac{\vartheta}{2},$$

from which we obtain (recall that $\theta \in (-\pi, \pi)$ and therefore $\cos(\vartheta/2) > 0$)

$$\frac{ds}{d\vartheta} = 2R\cos\frac{\vartheta}{2} \Longrightarrow s(\vartheta) = 4R\left[\sin\frac{\zeta}{2}\right]_0^{\vartheta} = 4R\,\sin\frac{\vartheta}{2}. \tag{7.34}$$

The expression of the metric in these coordinates is $g(\vartheta) = 2R\,\cos\frac{\vartheta}{2}\,d\vartheta^2$, i.e. the free motion is described by the Lagrangian with a position-dependent mass given by $m(\vartheta) = 2m_0\,R\,\cos\frac{\theta}{2}$: $L_0(\vartheta, \dot{\vartheta}) = m_0\,R\,\cos\frac{\vartheta}{2}\,\dot{\vartheta}^2$. The potential function describing the action of the gravity in terms of the arc-length s is:

$$V(\vartheta) = m_0\,\mathrm{g}\,y(\vartheta) = 2m_0\,\mathrm{g}\,R\,\sin^2\frac{\vartheta}{2} = 2m_0\,\mathrm{g}\,R\frac{s^2}{16R^2} = \frac{1}{2}\,m_0\,\frac{\mathrm{g}}{4R}\,s^2, \tag{7.35}$$

and then the Lagrangian is given by

$$L(\vartheta, \dot{\vartheta}) = m_0\,R\,\cos\frac{\vartheta}{2}\,\dot{\vartheta}^2 - 2m_0\,\mathrm{g}\,R\,\sin^2\frac{\vartheta}{2}, \tag{7.36}$$

or in terms of the canonical coordinate

$$L(s, \dot{s}) = \frac{1}{2}m_0\,\dot{s}^2 - \frac{1}{2}\,m_0\,\frac{\mathrm{g}}{4R}\,s^2. \tag{7.37}$$

Alternatively, as the tangent vector to the curve is

$$\mathbf{t}(\vartheta) = \frac{1}{2R\cos\frac{\vartheta}{2}}(R(1+\cos\vartheta), R\sin\vartheta) = \left(\cos\frac{\vartheta}{2}, \sin\frac{\vartheta}{2}\right),$$

then the tangential force is given by

$$F_t = \mathbf{F}\cdot\mathbf{t} = -m_0\,\mathrm{g}\sin\frac{\vartheta}{2} = -\frac{m_0\,\mathrm{g}}{4R}\,s,$$

while the tangential component of $\ddot{\mathbf{x}}$ is $\ddot{s}$, and then Newton's second law is

$$\ddot{s} = -\frac{m_0\,\mathrm{g}}{4R}\,s. \tag{7.38}$$

Both expressions (7.37) and (7.38) show that the motion along the inverted cycloid in terms of the arc-length s is oscillatory with a constant period function $\tau = \frac{2\pi}{\omega} = 4\pi\sqrt{\frac{R}{\mathrm{g}}}$. The initial position only fixes the amplitud of motion. This is the reason for the tautochronous behaviour of the motion along the cycloid [17, 18].

7.8 Quantisation of Motions on Curves

A curve is endowed with a (local) chart given by the arc-length which turns out to be a privileged chart. We can apply the usual canonical quantisation rule using such a chart because the expressions of the Lagrangian and Hamiltonian for free motion are exactly the same ones as for the Euclidean case, i.e.

$$L_0(s,\dot{s}) = \frac{1}{2} m_0 \dot{s}^2, \qquad H_0(s,p_s) = \frac{p_s^2}{2m_0}. \tag{7.39}$$

This means that a natural prescription is to replace the momentum p_s by $-i\,\hbar\partial/\partial s$ as an operator acting on the Hilbert space $\mathcal{L}_0^2(C, ds)$ of square integrable functions on the curve C vanishing on the boundary of C. As the measure ds is invariant under length-displacements such operator is selfadjoint.

As a particular instance we study the quantum model for a particle of mass m_0 living on a cycloid as configuration space, under the action of a gravitational force, in terms of the arc-length parameter is like that of a harmonic oscillator with mass m_0 and $\omega^2 = m_0\,\mathrm{g}/(4R)$, for $-4R \le s \le 4R$.

The Hilbert space of the corresponding quantum system will be $\mathcal{L}_0^2(-L, L)$ of square integrable functions in the interval $(-L, L)$, with $L = 4R$, satisfying the boundary conditions $\psi(-L) = \psi(L) = 0$, and the quantum Hamiltonian operator is given by

$$H = -\frac{\hbar^2}{2m_0}\frac{d^2}{ds^2} + V(s),$$

where

$$V(s) = \begin{cases} \frac{1}{2} m_0 \omega^2 s^2 & \text{if } |s| \le R \\ \infty & \text{if } |s| \ge 4R \end{cases}.$$

This problem of a confined harmonic oscillator has been studied by Ghosh [19]. The Hamiltonian is parity invariant and consequently the eigenfunctions are either even or odd functions. The time-independent Schrödinger equation is

$$\left(-\frac{\hbar^2}{2m_0}\frac{d^2}{ds^2} + \frac{1}{2} m_0 \omega^2 s^2\right)\psi(s) = E\,\psi(s),$$

which can be rewritten as

$$\frac{d^2}{dz^2} + \left(\varepsilon - \frac{z^2}{4}\right)\psi(z) = 0, \quad \text{where } z = \sqrt{\frac{2m_0\omega}{\hbar}} \text{ and } E = \varepsilon\,\hbar\omega.$$

It is common to write $\varepsilon = \nu + 1/2$, by similarity with the usual harmonic oscillator, i.e. $E = (\nu + 1/2)\,\hbar\omega$. If we introduce now the change $\psi(z) = e^{-z^2/4}\phi(z)$, and redefine the independent variable as $y = \frac{1}{2}z^2$, the new function $\phi(y)$ satisfies the confluent hypergeometric equation (see [20], p. 504):

$$y\frac{d^2\phi}{dy^2} + (b-y)\frac{d\phi}{dy} - a\,y = 0,$$

with $b = \frac{1}{2}$ and $a = -\frac{\nu}{2}$, i.e.

$$y\frac{d^2\phi}{dy^2} + \left(\frac{1}{2} - y\right)\frac{d\phi}{dy} + \frac{\nu}{2}\,y.$$

The point $y = 0$ is a regular singular point while $y = \infty$ is an irregular singularity. A basis of the linear space of solutions for $b \notin \mathbb{Z}$ is given by the confluent hypergeometric function, also called Kummer function $M(a, b, y)$ and its related function $U(a, b, y)$ with power expansions (see e.g. [20], p. 504):

$$M(a,b,y) = {}_1F_1(a,b,y) = \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n}\frac{y^n}{n!}$$
$$U(a,b,y) = \frac{\pi}{\sin(\pi b)}\left(\frac{M(a,b,y)}{\Gamma(1+a-b)\Gamma(b)} - y^{1-b}\frac{M(1+a-b,2-b,y)}{\Gamma(a)\Gamma(2-b)}\right)$$

where (a_n) denotes $(a_n) = a(a+1)\cdots(a+n-1)$, with $(a_0) = 1$.

The general solution $\psi(s)$ can be written as

$$\psi(s) = e^{-m\omega L^2/2\hbar}\left[\left(A + B\frac{\sqrt{\pi}}{\Gamma((1-\nu)/2)}\right)M\left(-\tfrac{\nu}{2}, \tfrac{1}{2}, \tfrac{m_0\omega s^2}{\hbar}\right)\right.$$
$$\left. -\ 2B\frac{\sqrt{\pi}}{\Gamma(-\nu/2)}\sqrt{\frac{m_0\omega}{\hbar}}\,s\,M\left(\tfrac{1-\nu}{2}, \tfrac{3}{2}, \tfrac{m_0\omega s^2}{\hbar}\right)\right].$$

The first term on the right-hand side is an even function and the second one is odd. Therefore, the conditions on the parameter ν for $\psi(s)$ to be an eigenfunction are

$$\left(A + B\frac{\sqrt{\pi}}{\Gamma((1-\nu)/2)}\right)M\left(-\tfrac{\nu}{2}, \tfrac{1}{2}, \tfrac{m_0\omega L^2}{\hbar}\right) = 0 \text{ for even functions,}$$
$$\frac{\sqrt{\pi}}{\Gamma(-\nu/2)}\sqrt{\frac{m_0\omega}{\hbar}}M\left(\tfrac{1-\nu}{2}, \tfrac{3}{2}, \tfrac{m_0\omega L^2}{\hbar}\right) = 0 \qquad \text{for odd functions.}$$

These equations should be used to determine the energy eigenvalues.

7.9 Quantisation of Position Dependent Mass Systems

The usual approach make use of the formalism (α, β, γ): T has the following expression introduced by von Roos [11] (generalizing a previous study by BenDaniel et al. [12]):

$$T_{\alpha\beta\gamma} = \frac{1}{4}\left(m^\alpha\, p\, m^\beta\, p\, m^\gamma + m^\gamma\, p\, m^\beta\, p\, m^\alpha\right), \quad \alpha+\beta+\gamma = -1\,. \tag{7.40}$$

We remark that in order to study a quantum system (in the Schrödinger picture) we should first fix the Hilbert space $\mathcal{H}$ and then the (essentially) selfadjoint operators corresponding to the relevant observables to be quantised. Therefore the quantisation of the Hamiltonian of a system means first to define the appropriate Hilbert space of pure states, and then construction of the quantum Hamiltonian.

In the problem of quantisation of a Hamiltonian system with a PDM the definition of the measure $d\mu$ defining the Hilbert space $L^2(\mathbb{R}, d\mu)$ strongly depends on the characteristics of the function $m(x)$. Note that the kinetic Lagrangian $L_0 = T$ for motion along a curve given by (7.31) admits an infinitesimal symmetry given by the vector field

$$X = \frac{\partial}{\partial s} = \frac{1}{\sqrt{f(u)}} \frac{\partial}{\partial u}, \tag{7.41}$$

which preserves the metric distance, because $\mathcal{L}_X(ds) = 0$.

In an analogous way, the kinetic Lagrangian $L_{g,0} = T_g$ for a position dependent mass system possesses an exact Noether symmetry. The function T_g is not invariant under translations but under the action of the vector field X given by [13]

$$X(x) = \frac{1}{\sqrt{m(x)}} \frac{\partial}{\partial x}, \tag{7.42}$$

(displacement $\delta x = \epsilon(m(x))^{-1/2}$, in the physicists language), i.e. we have $X^c(T) = 0$, where X^c denotes the tangent lift to the velocity phase space $\mathbb{R}\times\mathbb{R}$ (that, in differential geometric terms, is the tangent bundle TQ of the configuration space $Q = \mathbb{R}$) of the vector field $X \in \mathfrak{X}(\mathbb{R})$,

$$X^c(x, v) = \frac{1}{\sqrt{m(x)}} \left(\frac{\partial}{\partial x} - \left(\frac{1}{2} \frac{m'(x)}{m(x)} \right) v \frac{\partial}{\partial v} \right). \tag{7.43}$$

Recall that a Killing vector field $X \in \mathfrak{X}(M)$ in a Riemannian space (M, g), is a symmetry of the metric g, $\mathcal{L}_X g = 0$ and it also preserves the volume Ω_g determined by the metric, that is,

$$\Omega_g = \sqrt{|g|}\, dx^1 \wedge dx^2 \wedge \cdots \wedge dx^n, \qquad \mathcal{L}_X \Omega_g = 0,$$

where $|g|$ denotes the determinant of the matrix g defining the Riemann structure.

As mentioned above in (7.16), it has been shown in [9] that if $T_g(x, v) = \frac{1}{2} g_{ij}(x) v^i v^j$, then $X^c(T_g) = T_{\mathcal{L}_X g}$, and consequently, the above vector field X is a Killing vector field for g iff X^c is a symmetry for the associated kinetic energy function T_g. In fact it is a Killing vector field of the one-dimensional m-dependent metric $g = m(x)\, dx \otimes dx$, i.e. $ds^2 = m(x)\, dx^2$, because the line element is invariant under the flow of the vector field $X = f(x)\partial/\partial x$ when $f\, m' + 2\, m f' = 0$, and, therefore, in order to the vector field X to be a Killing vector, it should be proportional to the vector field (7.42), which represents (the infinitesimal generator of) an exact Noether symmetry for the geodesic motion. The 1-form θ_{T_g} is $\theta_{T_g} = m(x) v\, dx$, and the as-

sociated Noether constant of the motion P for the geodesic motion, called Noether momentum is $P = i\big(X^c\big)\,\theta_{T_g} = \sqrt{m(x)}\,v$.

The Hilbert space for a quantum system with a configuration space M is the linear space of square integrable functions on M with respect to an appropriate measure, $L^2(M\,,d\mu)$. It was shown in [13] that in the case of a natural system the measure to be considered must be invariant under the the Killing vector fields of the metric. Actually, given a transitive action $\Phi : G \times M \to M$ of a Lie group G on a differentiable manifold M, the associated quasi-regular representation is given by the action of G on the set of complex functions on M, $(U(g)\psi)(x) = \psi(\Phi(g^{-1}, x))$. If M admits a G-invariant measure $d\mu$ and we restrict the action to the set $L^2(M\,,d\mu)$, the representation so obtained is a unitary representation [13]. The fundamental vector field X_a, $a \in \mathfrak{g}$, which is given by

$$(X\psi)(x) = \frac{d}{dt}\psi(\Phi(\exp(-ta), x))_{|t=0},$$

is a first-order differential operator that when restricted to the subspace $L^2(M\,,d\mu)$ is a skew-selfadjoint operator provided that the measure μ is G-invariant. For the one-dimensional PDM system, the quantum system must be described by the Hilbert space $L^2(\mathbb{R}, d\mu_x)$ of square integrable functions with respect to a measure invariant under X, $d\mu_x$, therefore determined by the metric.

The invariance condition under $X = f(x)\partial/\partial x$ for the measure $d\mu_x = \rho(x)\,dx$ is $f\,\rho' + \rho f' = 0$. Then, the only measure invariant under X for $f(x) = (m(x))^{-1/2}$ is a multiple of $d\mu_x = \sqrt{m(x)}\,dx$.

This automatically implies that the first-order linear operator X is skew-symmetric and that the operator $\widehat{P}$ representing the quantum version of the Noether momentum P must be selfadjoint, not in the standard space $L^2(\mathbb{R}) \equiv L^2(\mathbb{R}, dx)$, but in the space $L^2(\mathbb{R}, d\mu_x)$ of square integrable functions with respect the PDM measure $d\mu_x$ [13].

Using Legendre transformation the momentum p and velocity v are related by $p = m(x)\,v$ and the expressions of Noether momentum and Hamiltonian (kinetic term plus a potential) in phase space are

$$P = \frac{1}{\sqrt{m(x)}}\,p\,, \quad \text{and} \quad H = \frac{1}{2}\,P^2 + V(x)\,. \tag{7.44}$$

As indicated in [13] the generator of the infinitesimal 'translation' symmetry', $(1/\sqrt{m(x)})\,d/dx$, is skew-Hermitian in the space $L^2(\mathbb{R}, d\mu_x)$ and therefore the transition from the classical system to the quantum one is given by defining the operator $\widehat{P}$ as follows

$$P \;\mapsto\; \widehat{P} = \frac{1}{\sqrt{m(x)}}\Big(-i\,\hbar\,\frac{d}{dx}\Big)\,, \tag{7.45}$$

so that

$$\frac{1}{m(x)}\,p^2 \;\to\; -\,\hbar^2\,\Big(\frac{1}{\sqrt{m(x)}}\,\frac{d}{dx}\Big)\Big(\frac{1}{\sqrt{m(x)}}\,\frac{d}{dx}\Big)\,,$$

in such a way that the quantum Hamiltonian $\widehat{H}$ is represented by the following Hermitian operator (defined on the space $L^2(\mathbb{R}, d\mu_x)$)

$$\widehat{H} = -\frac{\hbar^2}{2}\Big(\frac{1}{\sqrt{m(x)}}\,\frac{d}{dx}\Big)\Big(\frac{1}{\sqrt{m(x)}}\,\frac{d}{dx}\Big) + V(x) = -\frac{\hbar^2}{2}\,\frac{1}{m(x)}\,\frac{d^2}{dx^2} + \frac{\hbar^2}{4}\Big(\frac{m'(x)}{m^2(x)}\Big)\,\frac{d}{dx} + V(x)\,,$$

and then the Schrödinger equation $\widehat{H}\,\Psi = E\,\Psi$ becomes

$$-\frac{\hbar^2}{2}\,\frac{1}{m(x)}\,\frac{d^2\Psi}{dx^2} + \frac{\hbar^2}{4}\Big(\frac{m'(x)}{m^2(x)}\Big)\,\frac{d\Psi}{dx} + V(x)\Psi = E\,\Psi\,. \tag{7.46}$$

7.10 Constant Curvature Surfaces

As another example of quantisation of Noether momenta we consider the case of constant curvature surfaces. The expression of the arc-length element in geodesic polar coordinates (ρ, ϕ) on a constant cuvature surface M^2_κ can be written as follows

$$\begin{array}{ll} ds^2_\kappa = d\rho^2 + \frac{1}{\kappa}\sin^2(\sqrt{\kappa}\rho)\,d\phi^2\,, & \text{if } \kappa > 0,\\ ds^2_0 = d\rho^2 + \rho^2\,d\phi^2\,, & \text{if } \kappa = 0,\\ ds^2_\kappa = d\rho^2 - \frac{1}{\kappa}\sinh^2(\sqrt{-\kappa}\rho)\,d\phi^2\,, & \text{if } \kappa < 0. \end{array} \tag{7.47}$$

It is possible to deal with all of them in an unified way by introducing the following labelled trigonometric functions

$$\mathrm{C}_\kappa(x) = \begin{cases} \cos\sqrt{\kappa}\,x & \text{if } \kappa > 0,\\ 1 & \text{if } \kappa = 0,\\ \cosh\sqrt{-\kappa}\,x & \text{if } \kappa < 0, \end{cases} \qquad \mathrm{S}_\kappa(x) = \begin{cases} \frac{1}{\sqrt{\kappa}}\sin\sqrt{\kappa}\,x & \text{if } \kappa > 0,\\ x & \text{if } \kappa = 0,\\ \frac{1}{\sqrt{-\kappa}}\sinh\sqrt{-\kappa}\,x & \text{if } \kappa < 0, \end{cases} \tag{7.48}$$

and the κ-dependent tangent function $\mathrm{T}_\kappa(x) = \mathrm{S}_\kappa(x)/\mathrm{C}_\kappa(x)$. Fundamental properties of these curvature-dependent trigonometric functions and of their derivatives are

$$\mathrm{C}^2_\kappa(x) + \kappa\,\mathrm{S}^2_\kappa(x) = 1\,, \quad \mathrm{S}_\kappa(2x) = 2\mathrm{S}_\kappa(x)\mathrm{C}_\kappa(x)\,, \qquad \mathrm{C}_\kappa(2x) = \mathrm{C}^2_\kappa(x) - \kappa\mathrm{S}^2_\kappa(x)\,,$$

$$\frac{d}{dx}\mathrm{S}_\kappa(x) = \mathrm{C}_\kappa(x)\,, \qquad \frac{d}{dx}\mathrm{C}_\kappa(x) = -\kappa\mathrm{S}_\kappa(x)\,, \quad \frac{d}{dx}\mathrm{T}_\kappa(x) = \frac{1}{\mathrm{C}^2_\kappa(x)}.$$

With this notation the arc-length element in all the three cases is: $ds^2_\kappa = d\rho^2 + \mathrm{S}^2_\kappa(\rho)\,d\phi^2$, i.e. the only nonzero components of the metric are $g_{\rho\rho} = 1$, and $g_{\phi\phi} = \mathrm{S}^2_\kappa(\rho)$. Note that ρ denotes the distance along a geodesic on the manifold M^2_κ.

The Lagrangian for the geodesic (free) motion on the spaces $(S^2_\kappa, \mathbb{E}^2, H^2_\kappa)$ is

$$L_{0\kappa}(\rho, \phi, v_\rho, v_\phi) = T_\kappa(\rho, \phi, v_\rho, v_\phi) = \frac{1}{2}\left(v_\rho^2 + \mathrm{S}^2_\kappa(\rho) v_\phi^2\right), \tag{7.49}$$

and for a general mechanical type system (Riemannian metric minus a potential)

$$L_\kappa(\rho, \phi, v_\rho, v_\phi) = \frac{1}{2}\left(v_\rho^2 + \mathrm{S}^2_\kappa(\rho) v_\phi^2\right) - V(\rho, \phi, \kappa). \tag{7.50}$$

The corresponding Legendre transformation maps the point $(\rho, \phi, v_\rho, v_\phi)$ into $(\rho, \phi, p_\rho, p_\phi)$ with $p_\rho = v_\rho$, $p_\phi = \mathrm{S}^2_\kappa(\rho)\, v_\phi$, i.e. the Hamiltonian is

$$H = \frac{1}{2}\left(p_\rho^2 + \frac{p_\phi^2}{\mathrm{S}^2_\kappa(\rho)}\right) + V(\rho, \phi, \kappa). \tag{7.51}$$

Under the κ-dependent change of coordinates $r = \mathrm{S}_\kappa(\rho)$ the Lagrangian $L_{0\kappa}$ becomes

$$L_{0\kappa}(r, \phi, v_r, v_\phi) = \frac{1}{2}\left(\frac{v_r^2}{1 - \kappa\, r^2} + r^2 v_\phi^2\right), \tag{7.52}$$

and, if we define $x = r\, \cos\phi$ and $y = r\, \sin\phi$, the Lagrangian becomes

$$L_{0\kappa}(x, y, v_x, v_y) = \frac{1}{2}\, \frac{1}{1 - \kappa\, r^2}\Big[\, v_x^2 + v_y^2 - \kappa\, (x v_y - y v_x)^2\, \Big], \quad r^2 = x^2 + y^2\,. \tag{7.53}$$

The Hamiltonian expressed in terms of these coordinates can be found to be:

$$H_{0\kappa}(x, y, p_x p_y) = \frac{1}{2}\left(p_x^2 + p_y^2 - \kappa(x\, p_y - y\, p_x)^2\right). \tag{7.54}$$

In order to look for the Killing vector fields for the metric we recall that $X = X_\rho\, \partial/\partial\rho + X_\phi\, \partial/\partial\phi \in \mathfrak{X}(M^2_\kappa)$ is a Killing vector field if and only if its complete lift

$$X_\rho\, \frac{\partial}{\partial\rho} + X_\phi\, \frac{\partial}{\partial\phi} + \left(\frac{\partial X_\rho}{\partial\rho} v_\rho + \frac{\partial X_\rho}{\partial\phi}\, v_\phi\right) \frac{\partial}{\partial v_\rho} + \left(\frac{\partial X_\phi}{\partial\rho} v_\rho + \frac{\partial X_\phi}{\partial\phi}\, v_\phi\right) \frac{\partial}{\partial v_\phi}$$

is a strict symmetry of L, i.e. $X^c L = 0$. This implies that

$$\frac{\partial X_\rho}{\partial\rho} = 0, \qquad \frac{\partial X_\rho}{\partial\phi} + \mathrm{S}^2_\kappa(\rho)\, \frac{\partial X_\phi}{\partial\rho} = 0, \qquad \mathrm{S}_\kappa(\rho)\mathrm{C}_\kappa(\rho)\, X_\rho + \mathrm{S}^2_\kappa(\rho) \frac{\partial X_\phi}{\partial\phi} = 0.$$

A solution of this system is $X_\rho \equiv 0$ and $X_\phi = 1$, i.e. the vector field $X_3 = \partial/\partial\phi$. On the other side, as X_ρ only depends on ϕ, a simple derivation with respect to ϕ in the second equation leads to

$$\frac{\partial^2 X_\rho}{\partial\phi^2} + \mathrm{S}_\kappa^2(\rho)\frac{\partial^2 X_\phi}{\partial\rho\,\partial\phi} = 0,$$

while if we derive with respect to ρ in the expression obtained from the third equation

$$\frac{\partial X_\phi}{\partial\phi} = -\frac{\mathrm{C}_\kappa(\rho)}{\mathrm{S}_\kappa(\rho)}X_\rho,$$

we get

$$\frac{\partial^2 X_\phi}{\partial\rho\,\partial\phi} = \frac{1}{\mathrm{S}_\kappa^2(\rho)}X_\rho.$$

These relations show that X_ρ is a solution of the equation

$$\frac{\partial^2 X_\rho}{\partial\phi^2} + X_\rho = 0,$$

and then the value of X_ϕ may be then obtained from preceding relation. In summary, we have got the other two linearly independent Killing vector fields

$$X_1 = \cos\phi\frac{\partial}{\partial\rho} - \frac{\mathrm{C}_\kappa(\rho)}{\mathrm{S}_\kappa(\rho)}\,\sin\phi\frac{\partial}{\partial\phi}, \qquad X_2 = \sin\phi\frac{\partial}{\partial\rho} + \frac{\mathrm{C}_\kappa(\rho)}{\mathrm{S}_\kappa(\rho)}\,\cos\phi\frac{\partial}{\partial\phi}.$$

Note now that the vector fields X_1, X_2 and X_3 so defined are such that

$$[X_1, X_2] = -\kappa X_3, \quad [X_3, X_1] = -X_2, \quad [X_2, X_3] = -X_1,$$

and therefore they close on a real Lie algebra isomorphic either to $\mathfrak{so}(3)$, if $\kappa > 0$, $\mathfrak{so}(2,1)$, when $\kappa < 0$, or $\mathfrak{e}(2)$ when $\kappa = 0$, i.e. it depends on the value of κ.

The momentum map for this case is given by

$$\begin{aligned}
P_{\mathrm{H}1} &= -\theta_0(\bar{X}_1), \qquad P_1(\rho,\phi,p_\rho,p_\phi) = -p_\rho\,\cos\phi + p_\phi\,\frac{\mathrm{C}_\kappa(\rho)}{\mathrm{S}_\kappa(\rho)}\,\sin\phi\\
P_{\mathrm{H}2} &= -\theta_0(\bar{X}_2), \qquad P_2(\rho,\phi,p_\rho,p_\phi) = -p_\rho\,\sin\phi - p_\phi\,\frac{\mathrm{C}_\kappa(\rho)}{\mathrm{S}_\kappa(\rho)}\,\cos\phi\\
P_{\mathrm{H}3} &= -\theta_0(\bar{X}_3), \qquad P_3(\rho,\phi,p_\rho,p_\phi) = -p_\phi
\end{aligned}$$

The Hamiltonian of the corresponding free particle is

$$H(\rho,\phi,p_\rho,p_\phi) = \frac{1}{2}\,p_\rho^2 + \frac{p_\phi^2}{2\mathrm{S}_\kappa^2(\rho)},$$

which can be expressed in terms of the components of the momentum map (we use shorter notation P instead of P_{H}). From

$$\begin{pmatrix} P_1 \\ P_2 \end{pmatrix} = -\begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} p_\rho \\ p_\phi \dfrac{\mathrm{C}_\kappa(\rho)}{\mathrm{S}_\kappa(\rho)} \end{pmatrix},$$

we easily see that $P_1^2 + P_2^2 = p_\rho^2 + p_\phi^2 \dfrac{\mathrm{C}_\kappa^2(\rho)}{\mathrm{S}_\kappa^2(\rho)}$, and consequently, $P_1^2 + P_2^2 + \kappa P_3^2 = p_\rho^2 + p_\phi^2 \dfrac{1}{\mathrm{S}_\kappa^2(\rho)}$. This shows that the Hamiltonian can be written as $H = P_1^2 + P_2^2 + \kappa P_3^2$. Using Cartesian coordinates, $x = r\,\cos\phi$ and $y = r\,\sin\phi$, the Killing vector fields are:

$$X_1(\lambda) = \sqrt{1+\lambda r^2}\ \frac{\partial}{\partial x}\,, \quad X_2(\lambda) = \sqrt{1+\lambda r^2}\ \frac{\partial}{\partial y}\,, \quad X_3(\lambda) = x\,\frac{\partial}{\partial y} - y\,\frac{\partial}{\partial x}\,.$$

The conditions for a volume form $\mathrm{vol} = \varrho(x,y)\,dx \wedge dy$ to be invariant under such vector fields are:

$$\begin{aligned} &\sqrt{1+\lambda r^2}\,\frac{\partial \varrho}{\partial x}\,dx\wedge dy + \varrho\, d(\sqrt{1+\lambda r^2})\wedge dy \\ &\quad = \left(\sqrt{1+\lambda r^2}\,\frac{\partial \varrho}{\partial x} + \frac{\lambda\, x\, \varrho}{\sqrt{1+\lambda r^2}}\right) dx\wedge dy = 0\,, \\ &\sqrt{1+\lambda r^2}\,\frac{\partial \varrho}{\partial y}\,dx\wedge dy + \varrho\, dx\wedge d(\sqrt{1+\lambda r^2}) \\ &\quad = \left(\sqrt{1+\lambda r^2}\,\frac{\partial \varrho}{\partial y} + \frac{\lambda\, y\, \rho}{\sqrt{1+\lambda r^2}}\right) dx\wedge dy = 0\,, \end{aligned}$$

and therefore, y times the first equation minus x times the second one gives the invariance of the function ϱ under rotations $x\partial\varrho/\partial y - y\partial\varrho/\partial x = 0$, which implies: $\varrho(x,y) = f(r)$, with $r^2 = x^2 + y^2$, and when using such expression in the previous equations we obtain (for $r \neq 0$):

$$\sqrt{1+\lambda r^2}\,\frac{1}{r}\,\frac{df}{dr} + \frac{\lambda f}{\sqrt{1+\lambda r^2}} = 0 \Longleftrightarrow \frac{df}{f} = -\lambda \frac{r\,dr}{1+\lambda r^2}\,,$$

with general solution f proportional to $f(r) = (1+\lambda r^2)^{-1/2}$.

Natural mechanical systems involve a potential term. The two most studied situations are the harmonic oscillator and the Kepler-Coulomb system, that are the cases for constant curvature surface motions.

The harmonic oscillator on the unit sphere, on the Euclidean plane, or on the unit Lobachewski plane, arise as $V_\kappa(\rho) = \frac{1}{2}\,\alpha^2\,\mathrm{T}_\kappa^2(\rho)$, i.e. $V_1(\rho) = \frac{1}{2}\,\alpha^2\,\tan^2\rho$, $\quad V_0(\rho) = \frac{1}{2}\,\alpha^2\rho^2$, $\quad V_{-1}(\rho) = \frac{1}{2}\,\alpha^2\,\tanh^2\rho$. Now if we consider the κ-dependent change $\rho \to r = \mathrm{S}_\kappa(\rho)$ then the Lagrangian $L(\kappa)$ becomes

$$L(\kappa) = \frac{1}{2}\left(\frac{v_r^2}{1-\kappa r^2} + r^2 v_\phi^2\right) - \frac{1}{2}\alpha^2\left(\frac{r^2}{1-\kappa r^2}\right)$$

and, if we change to Cartesian coordinates, we arrive to

$$L(\kappa) = \frac{1}{2}\left(\frac{1}{1-\kappa r^2}\right)\Big[\, v_x^2 + v_y^2 - \kappa\,(x v_y - y v_x)^2\,\Big] - \frac{1}{2}\alpha^2\left(\frac{r^2}{1-\kappa r^2}\right),$$
$$r^2 = x^2 + y^2\,.$$

Similarly we can use these potential terms in the corresponding Hamiltonian.

As far as the Kepler-Coulomb system in constant curvature surface is concerned one uses $V_K(\rho) = -k/(\mathrm{T}_\kappa(\rho))$. In Cartesian coordinate, using that $\mathrm{C}_\kappa = \sqrt{1-\kappa\,\mathrm{S}_\kappa(\rho)}$,

$$V_K(r) = -\frac{k}{r}\sqrt{1-\kappa\,\mathrm{S}_\kappa(\rho)}.$$

7.11 Quantisation of Noether Momenta

In order to the differential operator be selfadjoint we need a Hilbert space $\mathcal{L}^2(Q, d\mu)$ such that the volume form be invariant under X_k, i.e. the Hilbert space of the quantisation must be $\mathcal{L}^2\left(Q, (1+\lambda r^2)^{-1/2}\, dx \wedge dy\right)$, and then the Killing vector fields $X_1(\lambda)$ and $X_2(\lambda)$ are skewsymmetric first order differential operators. This suggests us to quantise the momenta operators by associating the function P_k with $\widehat{P}_k = -\mathrm{i}\, X_k$:

$$\widehat{P}_x = -i\,\hbar\sqrt{1+\lambda r^2}\,\frac{\partial}{\partial x}\,, \qquad \widehat{P}_y = -i\,\hbar\sqrt{1+\lambda r^2}\,\frac{\partial}{\partial y}\,,$$

and then the quantum Hamiltonian for the free case is

$$\widehat{H} = -\frac{\hbar^2}{2m}\left((1+\lambda r^2)\frac{\partial^2}{\partial x^2} + \lambda x\frac{\partial}{\partial x}\right) - \frac{\hbar^2}{2m}\left((1+\lambda r^2)\frac{\partial^2}{\partial y^2} + \lambda y\frac{\partial}{\partial y}\right)$$
$$+\lambda\frac{\hbar^2}{2m}\left(x^2\frac{\partial^2}{\partial y^2} + y^2\frac{\partial^2}{\partial x^2} - 2xy\frac{\partial^2}{\partial x\,\partial y} - x\frac{\partial}{\partial x} - y\frac{\partial}{\partial y}\right)$$

which can be written as $\widehat{H} = \widehat{H}_1 + \widehat{H}_2 - \lambda\widehat{J}^2$, with

$$\widehat{H}_1 = -\frac{\hbar^2}{2m}\left((1+\lambda r^2)\tfrac{\partial^2}{\partial x^2} + \lambda x\tfrac{\partial}{\partial x}\right),$$
$$\widehat{H}_2 = -\frac{\hbar^2}{2m}\left((1+\lambda r^2)\tfrac{\partial^2}{\partial y^2} + \lambda y\tfrac{\partial}{\partial y}\right),$$
$$\widehat{J}^2 = -\frac{\hbar^2}{2m}\left(x^2\tfrac{\partial^2}{\partial y^2} + y^2\tfrac{\partial^2}{\partial x^2} - 2xy\tfrac{\partial^2}{\partial x\,\partial y} - x\tfrac{\partial}{\partial x} - y\tfrac{\partial}{\partial y}\right),$$

and each term commutes with the sum of the other two and therefore with $\widehat{H}$. Therefore we can consider three systems of compatible observables: $\{\widehat{H}_1, \widehat{H}_2 - \lambda J^2\}$, $\{\widehat{H}_1 - \lambda J^2, \widehat{H}_2\}$, and $\{\widehat{H}_1 + \widehat{H}_2, J\}$.

The case of harmonic oscillator includes a term $\frac{1}{2}\alpha^2 r^2(1-\kappa r^2)^{-1}$ and it was exhaustively analysed in [21–23] while the case of Kepler-Coulomb problem was analysed in [24] and in a recent paper [25].

Finally, let us remark that the computation of the Laplace–Beltrami operator corresponding to the given metric is very easy: the metric matrix is given by

$$(g_{ij}) = \frac{1}{1+\lambda r^2}\begin{pmatrix} 1+\lambda y^2 & -\lambda x y \\ -\lambda x y & 1+\lambda x^2 \end{pmatrix} \Longleftrightarrow (g^{ij}) = \begin{pmatrix} 1+\lambda x^2 & \lambda x y \\ \lambda x y & 1+\lambda y^2 \end{pmatrix},$$

and then, taking into account that $g = \det(g_{ij}) = (1+\lambda r^2)^{-1}$, the Laplace–Beltrami operator given by

$$\Delta\psi = |g|^{-1/2}\frac{\partial}{\partial x^i}\left(|g|^{1/2}\, g^{ij}\frac{\partial \psi}{\partial x^j}\right), \tag{7.55}$$

turns out to be:

$$\Delta = (1+\lambda x^2)\frac{\partial^2}{\partial x^2} + (1+\lambda y^2)\frac{\partial^2}{\partial y^2} + 2\lambda\left(x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y}\right) + 2\lambda x y\frac{\partial^2}{\partial x \partial y}. \tag{7.56}$$

7.12 Conclusions and Outlook

The existence of holonomic constraints leads to consider configuration spaces that are not open sets of $\mathbb{R}^n$ but more general differentiable manifolds, and then in order to do differential calculus in these manifolds local coordinates are used to make computations, but only intrinsic concepts, valid in any coordinate setting, are well defined. The observables of the classical theory are differentiable real functions but are only represented by functions of $\mathbb{R}^n$ once a coordinate system is fixed. This implies that concepts such as coordinates of position or momenta are only local and therefore the usual 'canonical quantisation prescription' does not work for these systems. We have proved that in simple cases of mechanical type systems, the use of Noether momenta corresponding to Killing symmetries can be useful to carry out the quantisation of such functions, and some Hamiltonians. The theory has been illustrated with simple but interesting examples, as one-dimensional position dependent mass systems, motion on curves and constant curvature surfaces.

The application of the quantisation procedure suggested in this paper to more cases will clarify the usefulness of the method. The main restriction of the method is that is based on the Lie algebra of Killing symmetries and this algebra may be too small. The extension of the theory to more general Hamiltonian system where there are magnetic terms is also to be studied and will be object of future work.

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Chapter 8
Conditions for Legitimate Memory Kernel Master Equation

Dariusz Chruściński

Abstract We provide conditions for the memory kernel governing time non-local quantum master equation which guarantee that the corresponding dynamical map is completely positive and trace-preserving. This approach gives rise to the new parametrization of dynamical maps in terms of two completely positive maps – so called legitimate pair. Actually, this new parameterizations is a natural generalization of Markovian semigroup. Interestingly our class contains recently studied models like semi-Markov evolution and collision models.

8.1 Introduction

In recent years the dynamics of open quantum systems is an active field of research [1–3]. Since any realistic physical system is never perfectly isolated from the external world (environment) it should be treated as an open one and hence the theory of open quantum systems plays the fundamental role for analyzing, modelling and controlling realistic quantum systems. It should be clear that open quantum systems are also fundamental for potential applications in modern quantum technologies such as quantum communication, cryptography and computation [4].

In this paper we concentrate on a proper mathematical description of quantum evolution which is represented by a family of completely positive trace-preserving maps $\Lambda_t : \mathscr{T}(\mathscr{H}) \to \mathscr{T}(\mathscr{H})$ $(t \geq 0)$, where $\mathscr{T}(\mathscr{H})$ denotes the Banach space of trace class operators with the trace norm defined by $||A||_1 = \mathrm{tr}|A|$. The natural initial condition at $t = 0$ reads $\Lambda_{t=0} = \mathrm{id}$. One calls such family a *dynamical map*. The map Λ_t maps an initial state represented by a density operator $\rho \in \mathscr{T}(\mathscr{H})$ into the state $\rho_t = \Lambda_t(\rho)$ at the current time $t > 0$. A natural framework for dynamical maps is the reduced evolution of a quantum system. Consider a composed system living

D. Chruściński (✉)
Institute of Physics, Faculty of Physics, Astronomy and Informatics,
Nicolaus Copernicus University, Grudziądzka 5/7, 87–100 Toruń, Poland
e-mail: darch@fizyka.umk.pl

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_8

in $\mathscr{H} \otimes \mathscr{H}_E$, where $\mathscr{H}_E$ denotes the Hilbert space of the environment. Fixing the initial state of the environment ρ_E one defines a map

$$\Lambda_t(\rho) := \mathrm{Tr}_E(U_t\, \rho \otimes \rho_E\, U_t^\dagger), \tag{8.1}$$

where $U_t = e^{-iHt}$, H stands for the Hamiltonian of the total (composed) system (throughout the paper we keep $\hbar = 1$), and Tr_E denotes the partial trace over environmental degrees of freedom. By construction the map Λ_t defined in (8.1) is completely positive and trace-preserving (CPTP). One calls Λ_t the reduced evolution of the system living in $\mathscr{H}$. It was proved by Nakajima and Zwanzig [5] that reduced evolution satisfies the following equation

$$\dot{\Lambda}_t = \int_0^t K_{t-\tau}\Lambda_\tau d\tau, \quad \Lambda_{t=0} = \mathrm{id}, \tag{8.2}$$

where the integral kernel K_t is a highly nontrivial function of the total Hamiltonian H and the initial state of the environment. One often calls (8.2) a *memory kernel master equation* and the operator $K_t : \mathscr{T}(\mathscr{H}) \to \mathscr{T}(\mathscr{H})$ a *memory kernel*. Note, that the rate of change of the map Λ_t at time t depends on its history (starting at $t = 0$).

In this paper we address the following problem: what are conditions for a memory kernel K_t such that the solution Λ_t of (8.2) provides a legitimate dynamical map, that is, Λ_t is CPTP for all $t \geq 0$. In the special case when $K_t = \delta(t)\mathscr{L}$ the memory kernel master equation (8.2) reduces to Markovian master equation

$$\dot{\Lambda}_t = \mathscr{L}\Lambda_t, \tag{8.3}$$

with $\mathscr{L}$ being the celebrated GKSL generator defined as follows [6, 7]

$$\mathscr{L}[\rho] = -i[H, \rho] + \sum_\alpha \gamma_\alpha (V_\alpha \rho V_\alpha^\dagger - \frac{1}{2}\{V_\alpha^\dagger V_\alpha, \rho\}), \tag{8.4}$$

where H denotes an effective Hamiltonian, V_α are noise operators, and $\gamma_\alpha \geq 0$ describe decoherence/dissipation rates. The evolution which goes beyond Markovian master equation (8.4) is often referred as non-Markovian evolution and is extensively analyzed in recent years (see e.g. recent reviews [8–11]).

The problem of necessary and sufficient conditions for K_t was already analyzed by many authors (see e.g. [12–21]). In this paper we follow recent approach proposed in [22] and analyzed recently in [23–25]. The main idea is to represent a dynamical map Λ_t in terms of two maps $\{N_t, Q_t\}$ which are completely positive but not trace-preserving. Suitable conditions guarantees that the resulting map Λ_t is both completely positive and trace-preserving. This construction enables one to find a large class of physically legitimate memory kernels.

8.2 Preliminaries

Let $\mathfrak{A}$ be a unital C^*-algebra. Recall that a linear map $\Phi : \mathfrak{A} \to \mathscr{B}(\mathscr{H})$ is positive iff $\Phi(a) \geq 0$ for any $a \geq 0$ ($a \geq 0$ iff $a = x^*x$ for some $x \in \mathfrak{A}$). A map Φ is k-positive if

$$\mathrm{id}_k \otimes \Phi : M_k(\mathbb{C}) \otimes \mathfrak{A} \to M_k(\mathbb{C}) \otimes \mathscr{B}(\mathscr{H}), \tag{8.5}$$

is positive ($M_k(\mathbb{C})$ denotes a matrix algebra of $k \times k$ complex matrices). Finally, Φ is completely positive (CP) if it is k-positive for all $k = 1, 2, \ldots$. One proves [26].

Proposition 1 *Φ is completely positive iff for any $a_1, \ldots, a_n \in \mathfrak{A}$ and $x_1, \ldots, x_n \in \mathscr{H}$*

$$\sum_{i,j=1}^{n} \langle x_i | \Phi(a_i^* a_j) | x_j \rangle \geq 0, \tag{8.6}$$

for all $n = 1, 2, \ldots$.

Due to the celebrated Stinespring representation [26, 27] any CP map $\Phi : \mathfrak{A} \to \mathscr{B}(\mathscr{H})$ may be represented as follows

$$\Phi(a) = V \pi(a) V^\dagger, \tag{8.7}$$

where $V : \mathscr{H} \to \mathscr{K}$ and $\pi : \mathfrak{A} \to \mathscr{B}(\mathscr{K})$ is a $*$-homomorphism ($\mathscr{K}$ is a Hilbert space).

In this paper we consider only finite dimensional case, i.e. linear maps $\Phi : L(\mathscr{H}) \to L(\mathscr{H})$, where $L(\mathscr{H})$ denotes linear operators acting on the finite dimensional Hilbert space $\mathscr{H}$. In this case $\mathscr{T}(\mathscr{H}) = \mathscr{B}(\mathscr{H}) = L(\mathscr{H})$ (considered as vector spaces). Recall that $\mathscr{T}(\mathscr{H})$ is a Banach space with the trace norm and $\mathscr{B}(\mathscr{H})$ is a C^*-algebra with the operator norm. In this case any CP map $\Phi : L(\mathscr{H}) \to L(\mathscr{H})$ is characterized by so called Kraus representation

$$\Phi(X) = \sum_{\alpha} K_\alpha X K_\alpha^\dagger, \tag{8.8}$$

where $K_\alpha \in L(\mathscr{H})$. The map is trace-preserving if the Kraus operators K_α satisfy $\sum_\alpha K_\alpha^\dagger K_\alpha = \mathbb{I}$. For any linear map $\Phi : L(\mathscr{H}) \to L(\mathscr{H})$ one defines its dual $\Phi^* : L(\mathscr{H}) \to L(\mathscr{H})$ via

$$\mathrm{Tr}(A\Phi(B)) = \mathrm{Tr}(\Phi^*(A)B),$$

for any $A, B \in L(\mathscr{H})$. A map Φ is trace-preserving iff its dual is unital, that is, $\Phi^*(\mathbb{I}) = \mathbb{I}$. Note, that if Φ is represented via (8.8) then its dual is also CP and its Kraus representation reads

$$\Phi^*(X) = \sum_\alpha K_\alpha^\dagger X K_\alpha. \tag{8.9}$$

A linear map $\Phi : L(\mathscr{H}) \to L(\mathscr{H})$ is Hermiticity-preserving (often called Hermitian) if $[\Phi(X)]^\dagger = \Phi(X^\dagger)$ for all $X \in L(\mathscr{H})$. It is well known [26, 27] that any positive map is necessarily Hermiticity-preserving.

8.3 Quantum Jump Representation of the Markovian Semigroup

Let us observe that any GKSL generator (8.4) may be represented as

$$\mathscr{L} = B - Z, \tag{8.10}$$

where the operators $B, Z : L(\mathscr{H}) \to L(\mathscr{H})$ are defined as follows:

$$B(\rho) = \sum_k V_k \rho V_k^\dagger \tag{8.11}$$

and

$$Z(\rho) = i(C\rho - \rho C), \tag{8.12}$$

with $C \in L(\mathscr{H})$ given by

$$C = H + \frac{i}{2} \sum_k V_k^\dagger V_k. \tag{8.13}$$

Evidently, B is a CP map. Moreover, its dual $B^* : L(\mathscr{H}) \to L(\mathscr{H})$ reads $B^*(X) = \sum_k V_k^\dagger X V_k$ and hence $B^*(\mathbb{I}) = \sum_k V_k^\dagger V_k$. Now, let us denote by N_t a solution of the following equation

$$\dot{N}_t = -ZN_t\,, \quad N_{t=0} = \mathrm{id}. \tag{8.14}$$

Proposition 2 *If $[B, Z] = 0$, then the solution to (8.3) reads*

$$\Lambda_t = N_t \sum_{k=0}^{\infty} \frac{t^k}{k!} B^k. \tag{8.15}$$

Proof One has

$$\Lambda_t = e^{t\mathscr{L}} = e^{t(B-Z)} = e^{-tZ} e^{tB} = N_t \sum_{k=0}^{\infty} \frac{t^k}{k!} B^k, \tag{8.16}$$

where we used $e^{X+Y} = e^X e^Y$ for commuting X and Y.

Note, that N_t is given by

$$N_t(\rho) = e^{-Zt}\rho = e^{-iCt}\rho e^{iC^\dagger t}, \tag{8.17}$$

and hence both $N_t = e^{-Zt}$ and e^{tB} are CP maps. It is, therefore, evident that Λ_t being the composition of two CP maps is CP as well. The map N_t is CP but it is not trace-preserving and hence the role of e^{tB} is to restore the trace preservation.

Proposition 3 *The map N_t is trace non-increasing.*

Proof One has for arbitrary density operator ρ

$$\frac{d}{dt}\mathrm{Tr}[N_t(\rho)] = \mathrm{Tr}[(-iC + iC^\dagger)\rho] = -\mathrm{Tr}[B^*(\mathbb{I})\rho] \leq 0, \tag{8.18}$$

due to $B^*(\mathbb{I}) \geq 0$.

Remark 1 A CP map $\Phi : L(\mathscr{H}) \to L(\mathscr{H})$ such that

$$\mathrm{Tr}[\Phi(\rho)] \leq \mathrm{Tr}\rho,$$

is often called a quantum operation [4].

Now, we generalize (8.15) to arbitrary B and Z, that is, we do not assume that B and Z commute.

Theorem 1 *The solution to (8.3) may be represented as follows*

$$\Lambda_t = N_t * \sum_{k=0}^{\infty} Q_t^{*n}, \tag{8.19}$$

where $X_t * Y_t := \int_0^t X_{t-\tau}Y_\tau d\tau$ denotes convolution, $Q_t := BN_t$, and $Q_t^{*n} := Q_t * \ldots * Q_t$ (n factors).

Proof Passing to the Laplace transform (LT) of (8.3) and (8.14) one finds

$$\widetilde{\Lambda}_s = \frac{1}{s - B + Z}, \quad \widetilde{N}_s = \frac{1}{s + Z} \tag{8.20}$$

and hence

$$\widetilde{\Lambda}_s = \widetilde{N}_s \frac{1}{\mathrm{id} - B\widetilde{N}_s}, \tag{8.21}$$

where $\widetilde{f}_s := \int_0^\infty f_t e^{-ts} dt$. Now, introducing $\widetilde{Q}_s := B\widetilde{N}_s$ one obtains

$$\widetilde{\Lambda}_s = \widetilde{N}_s \sum_{k=0}^{\infty} \widetilde{Q}_s^n, \tag{8.22}$$

which implies (8.19) in the time domain.

Note, that Formulae (8.20) allow also for another representation, that is, instead of (8.21) one equivalently has

$$\widetilde{\Lambda}_s = \frac{1}{\mathrm{id} - \widetilde{N}_s B} \widetilde{N}_s, \tag{8.23}$$

and hence introducing $P_t := N_t B$ one finds the following representation

$$\Lambda_t = \Big(\sum_{k=0}^{\infty} P_t^{*n} \Big) * N_t. \tag{8.24}$$

Using the definition of the convolution formula (8.24) may be rewritten as follows

$$\Lambda_t = \sum_{k=1}^{\infty} \int_0^t dt_k \int_0^{t_k} dt_{k-1} \ldots \int_0^{t_2} dt_1 N_{t-t_k} B N_{t_k - t_{k-1}} B \ldots B N_{t_2 - t_1}. \tag{8.25}$$

Remark 2 Note, that if $[B, Z] = 0$, then (8.19) and (8.24) reduce to (8.15). Indeed, one easily shows that $Q_t = P_t$, and

$$Q_t^{*n} = (BN_t)^{*n} = B^n N_t^{*n} = \frac{t^{n-1}}{(n-1)!} B^n N_t. \tag{8.26}$$

Remark 3 Representations (8.19) and (8.24) are often called a *quantum jump* representation of the dynamical map Λ_t and the CP map B is interpreted as quantum jump.

Remark 4 Representations (8.19) and (8.24) are complementary to the standard exponential representation of Markovian semigroup

$$\Lambda_t = e^{t\mathscr{L}} = \sum_{k=0}^{\infty} \frac{t^k}{k!} \mathscr{L}^k. \tag{8.27}$$

Note, that (8.27) immediately implies that Λ_t is trace-preserving but complete positivity is not evident. On the other hand, both (8.19) and (8.24) imply that Λ_t is CP but now the trace preservation is not evident. It shows that complete positivity and trace preservation are complementary properties.

8.4 A Class of Legitimate Memory Kernels

In this section we generalize the quantum jump representation of the Markovian semigroup to the solution of the memory kernel master equation (8.2). Any memory kernel K_t has the following general structure

$$K_t = B_t - Z_t, \tag{8.28}$$

where maps $B_t, Z_t : L(\mathscr{H}) \to L(\mathscr{H})$ are Hermitian and satisfy $\mathrm{Tr}[B_t(\rho)] = \mathrm{Tr}[Z_t(\rho)]$. This condition guarantees that K_t annihilates the trace, that is, $\mathrm{Tr}[K_t(\rho)] = 0$ for any ρ, and hence Λ_t is trace-preserving. Actually one easily proves the following

Proposition 4 *The solution to the memory kernel master equation (8.2) is trace-preserving iff the corresponding memory kernel K_t satisfies $\mathrm{Tr}[K_t(\rho)] = 0$ for any $\rho \in L(\mathscr{H})$.*

Remark 5 Note that defining a dual operator $K_t^* : L(\mathscr{H}) \to L(\mathscr{H})$ the annihilation of trace is equivalent to $K_t^*(\mathbb{I}) = 0$, that is, the dual operator annihilates identity operator $\mathbb{I} \in L(\mathscr{H})$. Clearly, it implies that the dual map Λ_t^* satisfies $\Lambda_t^*(\mathbb{I}) = \mathbb{I}$.

Theorem 2 *Let $\{N_t, Q_t\}$ be a pair of CP maps such that*

1. $N_{t=0} = \mathrm{id}$,
2. $\mathrm{Tr}[Q_t(\rho)] + \frac{d}{dt}\mathrm{Tr}[N_t(\rho)] = 0$ *for any* $\rho \in L(\mathscr{H})$,
3. $||\widetilde{Q}_s||_1 < 1$.

Then the following map

$$\Lambda_t = N_t * \sum_{n=0}^{\infty} Q_t^{*n}, \tag{8.29}$$

defines a legitimate dynamical map.

Proof Condition (3) guarantees that the series

$$\widetilde{\Lambda}_s = \widetilde{N}_s \sum_{k=0}^{\infty} \widetilde{Q}_s^n = \widetilde{N}_s \frac{1}{\mathrm{id} - \widetilde{Q}_s},$$

is convergent and hence (8.29) defines a CP map. Condition (1) implies that $\Lambda_{t=0} = N_{t=0} = \mathrm{id}$. Finally, condition (2) implies that the map Λ_t is trace-preserving. Indeed, passing the Laplace transform domain one finds

$$\mathrm{Tr}[\widetilde{Q}_s(\rho)] + \mathrm{Tr}[s\widetilde{N}_s(\rho) - \rho] = 0. \tag{8.30}$$

Now,

$$\widetilde{\Lambda}_s(\mathrm{id} - \widetilde{Q}_s) = \widetilde{N}_s, \tag{8.31}$$

and hence

$$\frac{1}{s}\mathrm{Tr}([\mathrm{id}-\widetilde{Q}_s](\rho))=\mathrm{Tr}[\widetilde{N}_s(\rho)), \tag{8.32}$$

due to

$$\mathrm{Tr}[\widetilde{\Lambda}_s(X)]=\frac{1}{s}\mathrm{Tr}\,X. \tag{8.33}$$

This proves that (8.30) is equivalent to the trace-preservation condition (8.32).

Remark 6 Note, that in the Heisenberg picture the trace-preservation condition is replaced by $\Lambda_t^*(\mathbb{I})=\mathbb{I}$ and it is equivalent to the following condition for the pair $\{N_t^*, Q_t^*\}$

$$Q_t^*(\mathbb{I})+\dot{N}_t^*(\mathbb{I})=0, \tag{8.34}$$

for all $t\geq 0$.

Remark 7 Note, that

$$\frac{d}{dt}\mathrm{Tr}[N_t(\rho)]=-\mathrm{Tr}[Q_t(\rho)]\leq 0, \tag{8.35}$$

for any density operator ρ due to the fact that Q_t is a CP map and hence $Q_t(\rho)\geq 0$. Hence, the map N_t is trace non-increasing (quantum operation).

Theorem 2 may be immediately generalized as follows

Corollary 1 *Let $\{N_t, Q_t\}$ be a pair of k-positive maps such that*

1. $N_{t=0}=\mathrm{id}$,
2. $\mathrm{Tr}[Q_t(\rho)]+\frac{d}{dt}\mathrm{Tr}[N_t(\rho)]=0$ *for any* $\rho\in L(\mathscr{H})$,
3. $||\widetilde{Q}_s||_1<1$.

Then the map $\Lambda_t=N_t*\sum_{n=0}^{\infty}Q_t^{*n}$ is k-positive and trace-preserving.

Actually, one may formulate the following

Corollary 2 *Let $\{N_t, P_t\}$ be a pair of CP maps such that*

1. $N_{t=0}=\mathrm{id}$,
2. $\mathrm{Tr}[P_t(\rho)]+\frac{d}{dt}\mathrm{Tr}[N_t(\rho)]=0$ *for any* $\rho\in L(\mathscr{H})$,
3. $||\widetilde{P}_s||_1<1$.

Then the following map

$$\Lambda_t=\sum_{n=0}^{\infty}P_t^{*n}*N_t, \tag{8.36}$$

defines a legitimate dynamical map.

In this case one has in the time domain

$$\Lambda_t = \sum_{k=1}^{\infty} \int_0^t dt_k \int_0^{t_k} dt_{k-1} \ldots \int_0^{t_2} dt_1 P_{t-t_k} P_{t_k-t_{k-1}} \ldots P_{t_3-t_2} N_{t_2-t_1}, \tag{8.37}$$

which generalizes (8.25).

Suppose now that $\{N_t, Q_t\}$ satisfy assumptions of Theorem 2 (i.e. conditions (1)–(3)). Moreover, let us assume that $\widetilde{N}_s$ is invertible. Then one proves the following

Theorem 3 *The operator $K_t = B_t - Z_t$, where*

$$\widetilde{B}_s = \widetilde{Q}_s \widetilde{N}_s^{-1}, \quad Z_s = \frac{\mathrm{id} - s\widetilde{N}_s}{\widetilde{N}_s}, \tag{8.38}$$

defines a legitimate memory kernel.

Proof Indeed, one has

$$\widetilde{\Lambda}_s = \frac{1}{s - \widetilde{B}_s + \widetilde{Z}_s}, \quad \widetilde{N}_s = \frac{1}{s + \widetilde{Z}_s} \tag{8.39}$$

which generalizes (8.20). Hence, the representation (8.29) easily follows.

Remark 8 This shows that knowing $\{N_t, Q_t\}$ one may construct a legitimate memory kernel. Following [23] we call $\{N_t, Q_t\}$ a *legitimate pair*.

To illustrate the above construction let us consider the following

Example 1 Let

$$N_t = \left(1 - \int_0^t f(\tau) d\tau\right) \mathrm{id}, \tag{8.40}$$

where the function $f : \mathbb{R}_+ \to \mathbb{R}$ satisfies:

$$f(t) \geq 0, \quad \int_0^{\infty} f(\tau) d\tau \leq 1.$$

Moreover, let $Q_t = f(t)\mathscr{E}$, where $\mathscr{E}$ is an arbitrary quantum channel. Then one finds the following formula for the memory kernel

$$K_t = \kappa(t)(\mathscr{E} - \mathrm{id}), \tag{8.41}$$

where the function $\kappa(t)$ is defined in terms of $f(t)$ as follows

$$\widetilde{\kappa}(s) = \frac{s\widetilde{f}(s)}{1 - \widetilde{f}(s)}. \tag{8.42}$$

In particular taking $f(t) = \gamma e^{-\gamma t}$ one finds $K_t = \delta(t)\mathscr{L}$, with

$$\mathscr{L} = \gamma(\mathscr{E} - \mathrm{id}), \tag{8.43}$$

being the GKSL generator.

8.5 Properties of Legitimate Pairs

Legitimate pairs $\{N_t, Q_t\}$ enjoy several interesting properties [23, 24].

Proposition 5 (Convexity) *If $\{N_t^{(k)}, Q_t^{(k)}\}$ are legitimate pairs then a convex combination $N_t = \sum_k p_k N_t^{(k)}$ and $Q_t = \sum_k p_k Q_t^{(k)}$ provide a legitimate pair.*

Proof It is evident that both N_t and Q_t are CP and $N_{t=0} = \mathrm{id}$. Moreover, the trace-preservation condition is easy to verify

$$\mathrm{Tr}[Q_t(\rho)] + \frac{d}{dt}\mathrm{Tr}[N_t(\rho)] = \sum_k p_k \left(\mathrm{Tr}[Q_t^{(k)}(\rho)] + \frac{d}{dt}\mathrm{Tr}[N_t^{(k)}(\rho)] \right) = 0.$$

Finally, observe that $||\widetilde{Q}_s||_1 \leq \sum_k p_k ||\widetilde{Q}_s^{(k)}||_1 \leq 1$ which guarantee convergence of $[\mathrm{id} - \widetilde{Q}_s]^{-1}$.

Proposition 6 (Reduced pair) *Suppose that $\{\mathbf{N}_t, \mathbf{Q}_t\}$ defines a legitimate pair for the evolution in $\mathscr{H} \otimes \mathscr{H}_E$. Then for arbitrary state ω in $\mathscr{H}_E$*

$$N_t(\rho) := \mathrm{Tr}_E(\mathbf{N}_t[\rho \otimes \omega]), \;\; Q_t(\rho) := \mathrm{Tr}_E(\mathbf{Q}_t[\rho \otimes \omega]),$$

provide a legitimate pair $\{N_t, Q_t\}$ corresponding to the Hilbert space $\mathscr{H}$.

Proof By construction N_t and Q_t are CP (reductions of CP maps $\mathbf{N}_t$ and $\mathbf{Q}_t$), and $N_{t=0} = \mathrm{id}$. Direct calculation easily verifies trace-preservation condition

$$\mathrm{Tr}[Q_t(\rho)] + \frac{d}{dt}\mathrm{Tr}[N_t(\rho)] = \mathrm{Tr}[\mathbf{Q}_t(\rho \otimes \omega)] + \frac{d}{dt}\mathrm{Tr}[\mathbf{N}_t(\rho \otimes \omega)] = 0,$$

which ends the proof.

Remark 9 This construction provides a straightforward generalization of

$$\Lambda_t(\rho) = \mathrm{Tr}_E(e^{-i\mathbf{H}t}\rho \otimes \omega e^{i\mathbf{H}t}), \tag{8.44}$$

corresponding to $\mathbf{B} = 0$. Note that Λ_t is a dynamical map whereas N_t is CP but it is not trace preserving. It should be stressed that the map Λ_t generated via the reduced pair $\{N_t, Q_t\}$ is not a reduction of the map generated by $\{\mathbf{N}_t, \mathbf{Q}_t\}$.

Proposition 7 (Gauge transformations) *If* $\{N_t, Q_t\}$ *is a legitimate pair,* $\mathscr{F}_t$ *is a dynamical map and* $\mathscr{G}_t$ *is a arbitrary CPTP map, then*

$$N'_t := \mathscr{F}_t N_t \ , \quad Q'_t := \mathscr{G}_t Q_t, \tag{8.45}$$

provide a legitimate pair as well.

Proof It is evident that N'_t and Q'_t are CP maps and $N'_{t=0} = \mathrm{id}$. The trace-preservation condition gives

$$\begin{aligned}\mathrm{Tr}[Q'_t(\rho)] + \frac{d}{dt}\mathrm{Tr}[N'_t(\rho)] &= \mathrm{Tr}[Q_t(\rho)] + \mathrm{Tr}[[\dot{\mathscr{G}}_t N_t + \mathscr{G}_t \dot{N}_t](\rho)] \\ &= \mathrm{Tr}[Q_t(\rho)] + \mathrm{Tr}[\dot{N}_t(\rho)] = 0,\end{aligned}$$

since $\mathscr{F}_t$ and $\mathscr{G}_t$ are trace-preserving and $\dot{\mathscr{G}}_t$ annihilates the trace.

Example 2 Taking N_t and Q_t as in Example 1 one obtains a new pair

$$N'_t = \left(1 - \int_0^t f(\tau)d\tau\right)\mathscr{F}_t \ , \quad Q'_t = f(t)\mathscr{G}_t. \tag{8.46}$$

In particular taking $\mathscr{F}_t = \mathscr{G}_t = e^{t\mathscr{L}}$, and $f(t) = \gamma e^{-\gamma t}$ one finds

$$\widetilde{N}'_s = \frac{1}{s + \gamma - \mathscr{L}} \ , \quad \widetilde{Q}'_s = \frac{\gamma}{s + \gamma - \mathscr{L}},$$

and hence the memory kernel reads

$$\widetilde{K}'_s = \widetilde{Q}'_s \widetilde{N}'^{-1}_s - (\mathrm{id} - s\widetilde{N}'_s)\widetilde{N}'^{-1}_s = \mathscr{L},$$

that is, the new kernel is purely local. This way we gauged away all memory effects already present in the original evolution governed by K_t.

Example 3 Consider a GKSL generator $\mathbf{L} = \mathbf{B} - \mathbf{Z}$ acting on $L(\mathscr{H} \otimes \mathscr{H}_E)$. Due to Proposition 6 for arbitrary state ω in $\mathscr{H}_E$

$$N(t)[\rho] = \mathrm{Tr}_E(e^{-\mathbf{Z}t}[\rho \otimes \omega]), \tag{8.47}$$

and

$$Q(t)[\rho] = \mathrm{Tr}_E(\mathbf{B}e^{-\mathbf{Z}t}[\rho \otimes \omega]), \tag{8.48}$$

provide a legitimate pair in $L(\mathscr{H})$. Clearly, in general $\{N(t), Q(t)\}$ no longer defines a semigroup (it defines a semigroup only if $\mathbf{Z} = Z \otimes \mathrm{id}_E$ and $\mathbf{B} = B \otimes \mathrm{id}_E$).

8.6 Non-homogeneous Memory Kernel Master Equation

Let us observe that any legitimate pair $\{N_t, Q_t\}$ gives rise to the following non-homogeneous memory kernel master equation

$$\dot{\Lambda}_t = \int_0^t K^{\rm new}_{t-\tau} \Lambda_\tau d\tau + \dot{N}_t \,, \tag{8.49}$$

where the new kernel $K^{\rm new}_t$ is defined in terms of LT as follows [23]

$$\widetilde{K}^{\rm new}_s = s\widetilde{N}_s \widetilde{Q}_s \widetilde{N}_s^{-1}, \tag{8.50}$$

that is, $\widetilde{K}^{\rm new}_s$ and $s\widetilde{Q}_s$ are related by a similarity transformation.

Remark 10 In particular if $[\widetilde{N}_s, \widetilde{Q}_s] = 0$, then

$$\widetilde{K}^{\rm new}_s = s\widetilde{Q}_s, \tag{8.51}$$

or equivalently in the time domain

$$K^{\rm new}_t = \dot{Q}_t + \delta(t) Q_0. \tag{8.52}$$

In this case (8.49) takes the following form

$$\dot{\Lambda}_t = Q_0 \Lambda_t + \int_0^t \dot{Q}_{t-\tau} \Lambda_\tau d\tau + \dot{N}_t. \tag{8.53}$$

Interestingly, this evolution is governed by three characteristic terms: local generator Q_0, time non-local kernel $\dot{Q}_t$, and non-homogeneous term $\dot{N}_t$. Integrating by parts in the second term one obtains

$$\dot{\Lambda}_t = \int_0^t Q_{t-\tau} \dot{\Lambda}_\tau d\tau + \dot{N}_t. \tag{8.54}$$

Example 4 Let us consider $\{N_t, Q_t\}$ as in Example 1. In this case $[N_t, Q_t] = 0$, and hence (8.53) reduces to the following one

$$\dot{\Lambda}_t = f(0) \mathscr{E} \Lambda_t + \int_0^t \dot{f}(t-\tau) \mathscr{E} \Lambda_\tau d\tau - f(t) {\rm id}, \tag{8.55}$$

or equivalently

$$\dot{\Lambda}_t = \int_0^t f(t-\tau) \mathscr{E} \dot{\Lambda}_\tau d\tau - f(t) {\rm id}, \tag{8.56}$$

Taking $f(t) = \Gamma e^{-\Gamma t}$, and the gauge $\mathscr{F}_t = \mathscr{G}_t$, one obtains

$$\dot{\Lambda}_t = \Gamma \int_0^t e^{-\Gamma(t-\tau)} \mathscr{E}\mathscr{F}_t \dot{\Lambda}_\tau d\tau + e^{-\Gamma t} \dot{\mathscr{F}}_t, \tag{8.57}$$

which recovers the memory kernel master equation derived in [28].

Example 5 Let us derive the non-homogeneous master equation for the Markovian semigroup. In this case one has (cf. Sect. 8.3)

$$N_t = e^{-Zt}, \quad Q_t = Be^{-Zt}.$$

One finds therefore the following equation for the dynamical map Λ_t

$$\dot{\Lambda}_t = B\Lambda_t - Z \int_0^t e^{-Z\tau} B \Lambda_{t-\tau} d\tau - Ze^{-Zt}. \tag{8.58}$$

Now, for the Markovian semigroup one has $\Lambda_t = e^{t(B_Z)}$ and hence inserting into (8.58) leads to the following identity

$$(B-Z)e^{(B-Z)t} = Be^{(B-Z)t} - Z \int_0^t e^{-Z\tau} Be^{(B-Z)(t-\tau)} d\tau - Ze^{-Zt}, \tag{8.59}$$

or after a simple algebra

$$Ze^{Zt} e^{(B-Z)t} = Z \int_0^t e^{Z\tau} Be^{(B-Z)\tau} d\tau + Z, \tag{8.60}$$

which is trivially satisfied if $[B, Z] = 0$. However, in the non-commutative case it is non-trivial and may be proved via the Baker-Campbell-Hausdorff formula.

8.7 Semi-Markov Evolution

In this section we analyze special class of legitimate pairs giving rise to so called quantum semi-Markov evolution [15, 18]. Let Q_t be a family of CP maps such that

$$\int_0^\infty Q_t^*(\mathbb{I}) dt \leq \mathbb{I}, \tag{8.61}$$

where Q_t^* denotes the dual map. One calls such map a *quantum semi-Markov map* [24]. Now, let us define so called quantum waiting time operator $\mathbf{f}_t := Q_t^*(\mathbb{I})$ and a quantum survival operator

$$\mathbf{g}_t := \mathbb{I} - \int_0^t \mathbf{f}_\tau d\tau. \tag{8.62}$$

Note, that if Q_t is quantum semi-Markov, then $\mathbf{g}_t \geq 0$. Finally, one defines N_t via

$$N_t(\rho) := \sqrt{\mathbf{g}_t}\,\rho\,\sqrt{\mathbf{g}_t}. \tag{8.63}$$

Proposition 8 *$\{N_t, Q_t\}$ defines a legitimate pair.*

Proof Clearly both maps are CP. Moreover $N_{t=0} = \mathrm{id}$ due to $\mathbf{g}_{t=0} = \mathbb{I}$. The trace-preservation condition (8.34) reads

$$Q_t^*(\mathbb{I}) + \dot{\mathbf{g}}_t = 0,$$

due to $\dot{\mathbf{g}}_t = -\mathbf{f}_t = -Q_t^*(\mathbb{I})$.

Let $|k\rangle$ $(k = 1, \ldots, d)$ denotes the orthonormal basis in $\mathscr{H}$ and let $e_{ij} := |i\rangle\langle j| \in L(\mathscr{H})$. Define a semi-Markov map Q_t by

$$Q_t(\rho) = \sum_{i,j=1}^{d} q_{ij}(t) e_{ij} \rho e_{ji}, \tag{8.64}$$

where $q_{ij}(t) \geq 0$. One finds

$$\mathbf{f}_t = Q_t^*(\mathbb{I}) = \sum_{i,j=1}^{d} q_{ij}(t) e_{ji} e_{ij} = \sum_{i,j=1}^{d} q_{ij}(t) e_{jj} =: \sum_{j=1}^{d} f_j(t) e_{jj}, \tag{8.65}$$

with $f_j(t) = \sum_{i=1}^{d} q_{ij}(t)$. Clearly, one finds for $\mathbf{g}_t$

$$\mathbf{g}_t = \sum_{j=1}^{d} g_j(t) e_{jj}, \tag{8.66}$$

with

$$g_t(t) = 1 - \int_0^t f_j(\tau) d\tau. \tag{8.67}$$

Hence, the map N_t has the following Kraus representation

$$N_t(\rho) = \sqrt{\mathbf{g}_t}\rho\sqrt{\mathbf{g}_t} = \sum_{i,j=1}^{d} \sqrt{g_i(t) g_j(t)}\, e_{ii}\, \rho\, e_{jj}. \tag{8.68}$$

This map represents the decoherence process with respect to the basis $|k\rangle$. Note, however, that it is not trace-preserving. Indeed, $\mathrm{Tr}[N_t(\rho)] = \sum_i g_i(t)\rho_{ii} \leq \mathrm{Tr}\rho$ due to $g_i(t) \leq 1$. The role of the additional map Q_t is to restore the trace-preservation. In

this case the whole evolution is controlled by a single map Q_t which is CP and satisfies additional constraint (8.61). Interestingly, this example is a mixture of classical map $q_{ij}(t)$ and the quantum map N_t representing trace non-increasing decoherence.

8.8 Conclusions

In this paper we provided a parametrization quantum dynamical maps in terms of pairs of CP maps $\{N_t, Q_t\}$ (or equivalently $\{N_t, P_t\}$). This construction provides a natural generalization of the parametrization for the Markovian semigroup, where the generator $\mathscr{L} = B - Z$ is related to the pair $\{N_t, Q_t\}$ via $N_t = e^{-Zt}$ and $Q_t = BN_t$. This approach is complementary to the time-local formulation base on the following master equation

$$\dot{\Lambda}_t = \mathscr{L}_t \Lambda_t \,, \quad \Lambda_{t=0} = \mathrm{id}, \tag{8.69}$$

where $\mathscr{L}_t$ denotes time-dependent local generator. In this case the solution is given by the Dyson series

$$\begin{aligned} \Lambda_t &= \mathscr{T} \exp\left(\int_0^t \mathscr{L}_\tau d\tau \right) \\ &= \mathrm{id} + \sum_{k=1}^{\infty} \int_0^t dt_k \int_0^{t_k} dt_{k-1} \ldots \int_0^{t_2} dt_1 \mathscr{L}_{t_k} \mathscr{L}_{t_{k-1}} \ldots \mathscr{L}_{t_1}, \end{aligned} \tag{8.70}$$

where $\mathscr{T}$ stands for time ordering operator. This series might be considered as complementary to (8.37). Both series control different properties: (8.37) controls complete positivity and (8.70) controls trace-preservation.

Finally, it should be stressed that our approach provides only a set of sufficient conditions which are in general not necessary. Finding these deserves further analysis. Such analysis is also needed in the case of time-local master equation (8.69) where only sufficient conditions for time local generator are known. It should be stressed that we considered only finite dimensional case. However, many results may be immediately generalized for infinite dimensions as well. It was already proved by Lindblad [7] that GKSL generator (8.4) works in the infinite dimensional case provided $\mathscr{L}$ is bounded. Recently, an unbounded generators for Markovian semi-groups were considered in [29]. One may also provide similar analysis for completely bounded [26] maps N_t and Q_t.

Acknowledgements This paper was partially supported by the National Science Center project 2015/17/B/ST2/02026.

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Chapter 9
From Classical Trajectories to Quantum Commutation Relations

F. M. Ciaglia, G. Marmo and L. Schiavone

Abstract In describing a dynamical system, the greatest part of the work for a theoretician is to translate experimental data into differential equations. It is desirable for such differential equations to admit a Lagrangian and/or an Hamiltonian description because of the Noether theorem and because they are the starting point for the quantization. As a matter of fact many ambiguities arise in each step of such a reconstruction which must be solved by the ingenuity of the theoretician. In the present work we describe geometric structures emerging in Lagrangian, Hamiltonian and Quantum description of a dynamical system underlining how many of them are not really fixed only by the trajectories observed by the experimentalist.

9.1 Introduction

When dealing with the description of a dynamical system in terms of differential equations, if we want to avoid the dry kind of approach: "Let M be a smooth manifold, and Γ a vector field on M", we should consider where this manifold comes from, how a vector field happens to exist on it and what is the relation of this vector field with the observation of an experimentalist. This analysis is an essential part of the

To Alberto on his 60th birthday.

F. M. Ciaglia
Max Planck Institute for Mathematics in the Sciences, Inselstrasse 22, 04103 Leipzig, Germany
e-mail: florio.ciaglia@mis.mpg.de

G. Marmo
Dipartimento di Fisica "E. Pancini", Università di Napoli Federico II, Complesso Universitario di Monte S. Angelo Edificio 6, via Cintia 80126, Napoli, Italy
e-mail: marmo@na.infn.it

L. Schiavone (✉)
Department of Mathematics, Faculty of Science, University of Ostrava, 30. dubna 22, 701 03 Ostrava, Czech Republic
e-mail: lucaschiavone@live.it

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_9

work of a theoretician. Interestingly enough, this point of view is already contained in one of Aristotele's observations [1]:

> Now, the path of investigation must lie from what is more intimately cognizable and clear to us, to what is clearer and more intimately cognizable in its own nature [...]
> So we must advance from the concrete data when we have analysed them [...]
> So we must advance from the concrete whole to the several constituents which it embraces [...]

Accordingly, we want to start with "what is more intimately cognizable and clear to us" in order to describe the dynamics of a generic dynamical system, that is, we want to start from a set of trajectories on some configuration space Q extracted from experimental data. We avoid here an epistemological digression about the construction of the configuration space from experimental data, and we refer to [2] for a detailed discussion.

In Sect. 9.2 we recall the main points of the construction of differential equations (in general implicit) from the set of experimental trajectories. In doing so, we shall see how the carrier manifold for the differential equation is something we should actively build out of experimental data, and not something that is there from the beginning. Then, assuming the resulting differential equation to be an explicit differential equation,[1] we pass to analyse the process of "tensorialization" of the Lagrangian and Hamiltonian description of the dynamics. Specifically, in Sect. 9.3 we consider the Lagrangian picture of classical mechanics, while in Sect. 9.4 we deal with the Hamiltonian picture. The tensorial characterization of the Lagrangian and Hamitlonian pictures allows us to clearly recognize the possibility of alternative Lagrangian and Hamiltonian descriptions for the same dynamical systems. Furthermore, we comment on the possibility of exploiting alternative tangent bundle structures on the same carrier manifold in order to obtain a Lagrangian description for dynamical systems that are not of second order with respect to a given tangent bundle structure. This could be particularly relevant in all of those situations in which it is necessary to reparametrize a given dynamics in order to obtain a complete vector field (e.g., the Kepler problem, see [3, 4]). In Sect. 9.5, we recall how the existence of alternative, nonlinearly related symplectic vector space structures on the same set allows for the definition of alternative and nonlinearly related quantum descriptions in terms of Weyl systems (an important example is provided by the so called F-OSCILLATORS, [5]).

9.2 Differential Equations from Experimental Data

We model the set $\mathcal{S}$ of observed trajectories as the set of curves over some configuration space subject to suitable regularity conditions:

$$\mathcal{S} = \{\gamma \mid \mathbb{I} \to Q \ : \ t \mapsto \gamma(t)\} \ . \tag{9.1}$$

[1] Some considerations on what happens when we obtain implicit differential equations are made in Appendix.

In general, curves in $\mathcal{S}$ intersect each others and we need to discriminate between intersecting curves if we want them to arise as solutions of first order differential equations. Essentially, we want to "lift" our curves from Q to a larger manifold where curves do not intersect anymore and may, possibly, be described as solutions of first order differential equations.

According to the results in [2], if we restrict our attention to Newtonian-like systems, that is, dynamical systems described by second order differential equations, on the configuration space, it is in general sufficient to lift the trajectories of the system from Q to the tangent bundle $\mathbf{T}Q$ to separate them. If this is not the case, that is, if trajectories lifted to the tangent bundle still intersect each other, successive lifting are not allowed because they will produce equations of motions of order greater than 2. Thus, in such a situation, one has to look for other ways to separate trajectories [2, 6]. More likely, trajectories furnished by the experimentalist belong to different dynamical systems, for instance they could be particles with different mass, different charge, different spin or some other characteristic property.

Let us limit our attention to the situation where the set

$$t\mathcal{S} = \{t\gamma \mid \mathbb{I} \to \mathbf{T}Q \ : \ t \mapsto (\gamma(t), \dot{\gamma}(t))\} \tag{9.2}$$

is a set of non-intersecting trajectories on $\mathbf{T}Q$. It is worth noting that, in general, the set $t\mathcal{S}$ may not coincide with the whole $\mathbf{T}Q$. In any case, it will be required to define a submanifold instead of just a subset of $\mathbf{T}Q$, if it does not coincide with the whole $\mathrm{T}Q$,

$$t\mathcal{S} = \mathcal{M} \subset \mathbf{T}Q\,. \tag{9.3}$$

In order to find the differential equation, it is possible to construct the set

$$tt\mathcal{S} = \{tt\gamma \mid \mathbb{I} \to \mathbf{TT}Q \ : \ t \mapsto (\gamma(t), \dot{\gamma}(t), \dot{\gamma}(t), \ddot{\gamma}(t))\}\ . \tag{9.4}$$

We require again that we are dealing with a submanifold of $\mathbf{TT}Q$

$$tt\mathcal{S} = \Sigma \subset \mathbf{TT}Q\,, \tag{9.5}$$

and, when some regularity conditions are satisfied ([2], Chap. 6), it may happen that Σ is the image of a second order vector field

$$\Gamma \mid \mathbf{T}Q \to \Gamma\,(\mathbf{TT}Q)\ . \tag{9.6}$$

This means that $\dot{\gamma}(t)$ and $\ddot{\gamma}(t)$ in (9.4) are given by the components of a second order vector field over $\mathbf{T}Q$. In this case it is possible to write the equations of motion for the dynamical system under investigation in the explicit form:

$$\dot{\gamma}(t) = \mathbf{v} \qquad \ddot{\gamma}(t) = f\,(\mathbf{q},\ \mathbf{v})\,, \tag{9.7}$$

where $(\mathbf{q},\ \mathbf{v})$ are coordinates on $\mathbf{T}Q$.

Remark 1 There are situations in which the submanifold $\Sigma \subset \mathbf{T}\mathbf{T}Q$ can not be written as the image of a second order vector field over $\mathbf{T}Q$. Then, $\Sigma \subset \mathbf{T}\mathbf{T}Q$ may be interpreted as an implicit differential equation over $\mathbf{T}Q$ ([7], Sect. 5). It may also happen that by the lifting procedure we do not cover all of $\mathbf{T}Q$ but only a subset, in this case we would say that our system is subject to some non-holonomic constraints. This would be the case, for instance, when we describe a relativistic particle with Q being the space-time.

In physics it is found convenient to ask for a description of the equations of motion in terms of some suitable function, both to be able to exploit Noether's theorem and to deal with quantization procedures. In this regard, two possibilities have proven to be quite satisfactory: the LAGRANGIAN and the HAMILTONIAN pictures. In the former case, the function, also called the LAGRANGIAN FUNCTION, is a real-valued function $\mathscr{L} \mid \mathbf{T}Q \to \mathbb{R}$ on the tangent bundle of the configuration space Q giving rise to the following differential equations on $\mathbf{T}Q$, the so called EULER- LAGRANGE EQUATIONS:

$$\begin{aligned} \frac{d}{dt}\frac{\partial \mathscr{L}}{\partial v^j} - \frac{\partial \mathscr{L}}{\partial q^j} &= 0 \\ \frac{d}{dt}q^j - v^j &= 0\,. \end{aligned} \tag{9.8}$$

They are clearly implicit differential equations. Indeed, by expanding the time derivatives, one has:

$$\frac{\partial^2 \mathscr{L}}{\partial v^i \partial v^j}\,\dot{v}^j + \frac{\partial^2 \mathscr{L}}{\partial v^i \partial q^j}\,v^j - \frac{\partial \mathscr{L}}{\partial q^i} = 0 \tag{9.9}$$

with $v^i = \frac{dq^i}{dt}$, where it is clear that the equation may be reduced to an explicit one only if the matrix $\frac{\partial^2 \mathscr{L}}{\partial v^i \partial v^j}$ is invertible, that is, if the Lagrangian is non-degenerate. From the geometrical point of view, the specific form of these equations requires the carrier space to possess a tangent bundle structure.[2]

In the latter case the function is a real-valued function on the cotangent bundle $\mathscr{H} \mid \mathbf{T}^*Q \to \mathbb{R}$, also called the HAMILTONIAN FUNCTION, giving rise to HAMILTON EQUATIONS:

$$\frac{d}{dt}q^i = -\frac{\partial \mathscr{H}}{\partial p_i} \qquad \frac{d}{dt}p_i = \frac{\partial \mathscr{H}}{\partial q^i}\,. \tag{9.10}$$

Quite clearly, these equations are always explicit differential equations, independently of the form and properties of $\mathscr{H}$. As we will explain later in this section, in this Hamiltonian case, the fundamental geometrical structure is the so called LIOUVILLE ONE FORM, θ, which defines the partial linear structure of the cotangent bundle in a canonical way [11] and whose differential is the canonical symplectic

[2] Other approaches, that are useful for dealing with explicitly time-dependent systems, take as fundamental structure the first order jet bundle of the Cartesian product $\mathbb{R} \times Q$, $\mathbf{J}^1(\mathbb{R} \times Q)$, and as Lagrangian, an horizontal density over such a fiber bundle ([8], Sect. 4.1, [9], Chaps. 3 and 4, and [10], Chap. 3, p. 97).

form ω on the cotangent bundle $\mathbf{T}^*Q$, that is, a closed, non-degenerate 2-form on $\mathbf{T}^*Q$. In a coordinates system $(\mathbf{q}, \mathbf{p})$ adapted to the cotangent bundle structure of $\mathbf{T}^*Q$, the LIOUVILLE ONE FORM reads $\theta = p_j \mathrm{d}q^j$, while the symplectic form reads $\omega = \mathrm{d}p_j \wedge \mathrm{d}q^j$ and the partial linear structure is $\Delta = p_i \frac{\partial}{\partial p_i}$.

Remark 2 The problem of finding a Lagrangian or an Hamiltonian and a Poisson structure such that the equations of motion found in the previous section by means of experimental data coincide with Euler-Lagrange or Hamilton equations is a non-trivial problem in Mathematics. It is, in fact, probably one of the most important problems in the Calculus of Variations and it is the so called INVERSE PROBLEM OF THE CALCULUS OF VARIATIONS.

Regarding the Lagrangian formalism, in the "lucky case" where equations of motion are explicit differential equations, a (non-unique) solution is known, provided that some conditions, the so-called HELMHOLTZ CONDITIONS, are satisfied.[3] For fair implicit differential equations, the inverse problem is in general not widely studied (see however [16, 17]), and we refer to Appendix for a discussion about the difficulties in formulating the problem.

In the Hamiltonian case, the problem is slightly more complicated because we should be looking for both a Hamiltonian and a Poisson structure at the same time. The existence of a possible Poisson description, according to Dirac, seems to be a necessary condition to carry on a quantization procedure [18].

9.3 Dynamical Systems and Geometrical Structures: Lagrangian Picture

A great boost in our understanding of the Lagrangian and Hamiltonian formalisms mentioned above came when a tensorial characterization of the fundamental geometric structures underlying these descriptions of the dynamics was achieved. Regarding the Lagrangian formulation of dynamics, a necessary step in the "tensorialization" process is a tensorial characterization of the structure of tangent bundle and second order (Newtonian-like) vector fields (as given for instance in [19]). Essentially, given a smooth manifold of dimension $2n$, say $\mathcal{M}$, a tangent bundle structure for $\mathcal{M}$ is encoded in the following two objects:

- a $(1, 1)$ tensor field, say S, such that $S^2 = 0$, $Ker\, S = Im\, S$ and $\mathcal{N}_S = 0$, where $\mathcal{N}_S$ denotes the Nijenhuis tensor associated with S ([13], Sect. 2.4);
- a partial linear structure Δ (see Definition 3.15 at p. 158 in [11]), whose critical points constitute a smooth submanifold of $\mathcal{M}$ of dimension n, and such that $\mathcal{L}_\Delta S = -S$ and $S(\Delta) = 0$.

We do not give a proof of the theorem for which we refer to [19]. However, the condition $Ker\, S = Im\, S$ tells us that $\mathcal{M}$ is even-dimensional and then the whole proof

[3] See [12] for an analytic introduction, [13, 14] for a geometrical approach on the tangent bundle and [8, 9, 15] for an approach on jet bundles and for an introduction to Variational Sequences.

is based on the construction of an atlas over $\mathcal{M}$ in which S and Δ take, in a local chart of such an atlas, their "canonical" form:

$$S = \frac{\partial}{\partial v^i} \otimes dq^i \qquad \Delta = v^i \frac{\partial}{\partial v^i}\,, \tag{9.11}$$

where the q^j's may be then interpreted as configuration-like coordinates, while the v^j may be interpreted as velocity-like coordinates, and we have $\mathcal{M} \cong TQ$. Then, it is clear that the only diffeomorphisms preserving the given tangent bundle structure encoded in Δ and S are all those diffeomorphisms $\Phi\colon \mathcal{M} \to \mathcal{M}$ that are the tangent lift $T\phi$ of some diffeomorphism $\phi\colon Q \to Q$. Locally, these diffeomorphisms may always be written as:

$$q'^i = f^i(\mathbf{q}) \qquad v'^i = v^j \frac{\partial f^i}{\partial q^j}\,. \tag{9.12}$$

In this sense, S and Δ represent the tangent bundle structure and identify the subgroup of diffeomorphisms which preserve them both.

In this framework, a second order (Newtonian-like) vector field Γ on $\mathbf{T}Q \cong \mathcal{M}$ is defined as a vector field the integral curves (on $\mathbf{T}Q \cong \mathcal{M}$) of which are tangent lifts of curves on the base manifold Q. It is easy to see that, in every coordinate system $(\mathbf{q}, \mathbf{v})$ which is adapted to the tangent bundle structure on $\mathbf{T}Q \cong \mathcal{M}$ encoded in S and Δ, the second order (Newtonian-like) vector field Γ can be written as:

$$\Gamma = v^j \frac{\partial}{\partial q^j} + \Gamma^j(q, v) \frac{\partial}{\partial v^j}\,. \tag{9.13}$$

From this it is possible to give a purely tensorial description of a second order vector field in terms of S and Δ as follows

$$S(\Gamma) = \Delta\,. \tag{9.14}$$

This tensorial characterization of second order (Newtonian-like) vector fields allows us to immediately see what happens to the second order vector field Γ when we perform arbitrary transformations on the manifold $\mathcal{M} \cong \mathbf{T}Q$. Consequently, let us consider a diffeomorphism $\phi\colon \mathcal{M} \to \mathcal{M}$ which is not necessarily adapted to the tangent bundle structure on $\mathcal{M}$ encoded in S and Δ. Since ϕ is a diffeomorphism, it is possible to transform Γ by means of ϕ to obtain another vector field on $\mathcal{M}$. Then, we may look at what happens to (9.14) under the action of ϕ obtaining:

$$\phi_* [S(\Gamma)] = \phi_* \Delta \quad \to \quad \left(\phi^* S\right) (\phi_* \Gamma) = \phi_* \Delta\,. \tag{9.15}$$

This equation is interpreted as the SODE condition for the "transformed" field, $\phi_* \Gamma$ with respect to the "transformed" tangent bundle structure given by $\phi^* S$ and $\phi_* \Delta$. From this, it follows that an arbitrary transformation on $\mathcal{M}$ will transform our vector field into a vector field which is still a second order vector field, but, in general, with

respect to another alternative tangent bundle structure on $\mathcal{M}$. In particular, when ϕ is a symmetry for Γ, that is, if $\phi_* \Gamma = \Gamma$, we obtain:

$$\left(\phi^* S\right) \Gamma = \phi_* \Delta \,, \tag{9.16}$$

which means that the vector field Γ itself is a second order vector field also for the alternative tangent bundle structure given by $\phi^* S$ and $\phi_* \Delta$.

The notion of second-order vector field, together with the tensorial characterization of the tangent bundle structure encoded in S and Δ, allows to give a tensorial formulation of the Euler-Lagrange equations. Given the Lagrangian function $\mathscr{L}$, we define the 1-form:

$$\theta_{\mathscr{L}} \;:=\; \mathrm{d}_S \mathscr{L} \,, \tag{9.17}$$

where d_S is defined as $\mathrm{d}_S \;:=\; S \circ \mathrm{d}$ according to formula (2.4.12) at p. 170 [13], and its action on functions reads $S \circ \mathrm{d}$. The one-form $\theta_{\mathscr{L}}$ is a semi-basic form on $\mathbf{T}Q$, and its coordinate expression in a coordinates system $(\mathbf{q},\ \mathbf{v})$ adapted to the tangent bundle structure of $\mathbf{T}Q$ reads:

$$\theta_{\mathscr{L}} = \frac{\partial \mathscr{L}}{\partial v^i}\, dq^i \,. \tag{9.18}$$

Now, we may introduce the so-called Lagrangian 2-form:

$$\omega_{\mathscr{L}} \;:=\; -\mathrm{d}\, \theta_{\mathscr{L}} \,. \tag{9.19}$$

This is a closed 2-form on $\mathbf{T}Q$, and we may consider the equation:

$$i_\Gamma\, \omega_{\mathscr{L}} \;=\; \mathrm{d} E_{\mathscr{L}} \,, \tag{9.20}$$

where Γ is a vector field on $\mathbf{T}Q$ and $E_{\mathscr{L}} := \Delta(\mathscr{L}) - \mathscr{L}$. In general, this equation does not admit of a unique solution. Indeed, if the two-form is degenerate it may happen that there is no solution and when a solution exists it need not be unique. However, if $\omega_{\mathscr{L}}$ is non-degenerate,[4] then it is a symplectic form and (9.20) admits a unique solution Γ which is a second-order vector field on $\mathbf{T}Q$. Using the CARTAN'S IDENTITY (i.e., $\mathcal{L}_X = i_X\, \mathrm{d} + \mathrm{d}\, i_X$) it is possible to show that (9.20) is equivalent to

$$\mathcal{L}_\Gamma\, \theta_{\mathscr{L}} - \mathrm{d}\mathscr{L} = 0 \,. \tag{9.21}$$

Furthermore, it is easy to see that, in a coordinates system $(\mathbf{q},\ \mathbf{v})$ adapted to the tangent bundle structure of $\mathbf{T}Q$, (9.21) acquires the usual Euler-Lagrange form:

$$\frac{d}{dt} \frac{\partial \mathscr{L}}{\partial v^j} - \frac{\partial \mathscr{L}}{\partial q^j} = 0 \,. \tag{9.22}$$

[4] Nondegenerancy of $\omega_{\mathscr{L}}$ is equivalent to $\det(\frac{\partial^2 \mathscr{L}}{\partial v^j \partial v^k}) \neq 0$ ([13], Sect. 3). When this is not the case, a careful analysis of the given situation is needed since, in general, we are in the presence of the description of a physical system in terms of fair implicit differential equations.

Now that we have a tensorial formulation of Euler-Lagrange equations, we may consider some diffeomorphism ϕ on $\mathcal{M} \cong \mathbf{T}Q$ and look at the "transformation properties" of Euler-Lagrange equations. We will do it by looking at how the differential 1-form on the left hand side of (9.21) changes by taking its pull-back trough the diffeomorphism ϕ. By using Theorem 7.4.4 at p. 413 and Proposition 7.4.10 at p. 416 in [20], and by using the CARTAN'S IDENTITY for the Lie derivative, we have

$$\mathcal{L}_{\phi^*\Gamma}\, \phi^*\theta_{\mathscr{L}} - \mathrm{d}\, \phi^*\mathscr{L} = 0 \tag{9.23}$$

Again, if ϕ is the tangent lift of a diffeomorphism on Q (i.e., $\phi = T\varphi$ for some $\varphi : Q \to Q$), and when it is a symmetry for Γ (i.e., $\phi^*\Gamma = \Gamma$), we obtain different Lagrangian descriptions for the same dynamical system. For a complete geometrical characterization of alternative Lagrangian descriptions we refer to [13].

Remark 3 Until now, we have always started with a vector field which is of second order with respect to some tangent bundle structure on $\mathcal{M}$. However, we may think of starting with a generic vector field which is not a second order one and ask if and how it is possible to "transform" it into a second order one with respect to some yet undetermined tangent bundle structure on $\mathcal{M}$ (if it exists). In particular, given a vector field Γ over the tangent bundle of some configuration space Q, say $\mathcal{M} \cong \mathbf{T}Q$, characterized by S and Δ, we may ask if it is possible to endow $\mathcal{M}$ with an alternative tangent bundle structure which makes the given vector field into a second order one. We will now write down some simple examples of such a situation in a coordinate-dependent fashion, postponing a tensorial analysis to a future work.

Example Let us consider a configuration space $Q \cong \mathbb{R}$. Then $\mathbf{T}Q \cong \mathbf{T}\mathbb{R} \cong \mathbb{R}^2$. Consider a coordinatization $(q,\ v)$ over $\mathbf{T}Q$ and the vector field:

$$\Gamma = f(v) v \frac{\partial}{\partial q} \tag{9.24}$$

where f is a nowhere vanishing function and $\mathrm{d}(f(v)\, v) \neq 0$. This vector field would describe a reparametrized free particle with a reparametrization-function which is a constant of the motion. We may need a more general reparametrization if we want to turn a vector field into a complete one (this would be the case for the Kepler problem. See [3]). Now, consider a diffeomorphism:

$$\phi \mid \mathbf{T}Q \to \mathbf{T}Q \ : \ (q,\ v) \mapsto (\phi_1(q,\ v) =: y,\ \phi_2(q,\ v) =: w) \tag{9.25}$$

then we can transform Γ through ϕ^{-1}:

$$\left(\phi^{-1}\right)_* \Gamma = f(v) v \left(\frac{\partial y}{\partial q} \frac{\partial}{\partial y} + \frac{\partial w}{\partial q} \frac{\partial}{\partial w} \right) \tag{9.26}$$

Looking at the previous expression, in order to obtain a second order vector field, we need a diffeomorphism such that:

$$f(v)v\frac{\partial y}{\partial q} = w \tag{9.27}$$

It is easy to see that if we consider the following diffeomorphism:

$$y = \frac{q}{f(v)} \qquad w = v \tag{9.28}$$

then:

$$\left(\phi^{-1}\right)_* \Gamma = w\frac{\partial}{\partial y} \tag{9.29}$$

which is a second order vector field with respect to the tangent bundle structure characterized by:

$$S' = \mathrm{d}y \otimes \frac{\partial}{\partial w} \qquad \Delta' = w\frac{\partial}{\partial w} \tag{9.30}$$

Example Now, let us consider the following vector field on $\mathbf{T}\mathbb{R}$:

$$\Gamma = \omega\, v\frac{\partial}{\partial q} - \omega\, q\frac{\partial}{\partial v} \tag{9.31}$$

where ω is a constant of the motion for Γ. This is again a reparametrized vector field with a reparametrization function which is a constant of the motion. Consider, again a diffeomorphism:

$$\phi \mid \mathbf{TQ} \to \mathbf{TQ} \ : \ (q,\, v) \mapsto (\phi_1(q,\, v) =: y,\, \phi_2(q,\, v) =: w) \tag{9.32}$$

and let us evaluate the following vector field:

$$\left(\phi^{-1}\right)_* \Gamma = \omega\left(v\frac{\partial y}{\partial q} - q\frac{\partial y}{\partial v}\right)\frac{\partial}{\partial y} + \omega\left(v\frac{\partial w}{\partial q} - x\frac{\partial w}{\partial v}\right)\frac{\partial}{\partial w} \tag{9.33}$$

then it is a matter of direct computation to show that, if one takes:

$$y = \frac{q}{\omega^2} \qquad w = \frac{v}{\omega} \tag{9.34}$$

then:

$$\left(\phi^{-1}\right)_* \Gamma = w\frac{\partial}{\partial y} - \omega^2 y\frac{\partial}{\partial w} \tag{9.35}$$

which is a second order vector field with respect to the tangent bundle structure given by:

$$S' = \mathrm{d}y \otimes \frac{\partial}{\partial w} \qquad \Delta' = w\frac{\partial}{\partial w} \tag{9.36}$$

and which represent an harmonic oscillator of frequency ω, where the frequency is a constant of the motion, it is an example of F- OSCILLATOR (see [5]).

Example Now, let us consider the following vector field on $\mathbf{T}\mathbb{R}$:

$$\Gamma = q\frac{\partial}{\partial q} \tag{9.37}$$

By means of a diffeomorphism, as in the previous two examples, one has:

$$\left(\phi^{-1}\right)_* \Gamma = q\left(\frac{\partial y}{\partial q}\frac{\partial}{\partial y} + \frac{\partial w}{\partial q}\frac{\partial}{\partial w}\right) \tag{9.38}$$

Here, it is easy to show that if one takes the following diffeomorphism:

$$y = q + f(v) \qquad w = q \tag{9.39}$$

with $\mathrm{d}f \wedge \mathrm{d}q \neq 0$, then:

$$\left(\phi^{-1}\right)_* \Gamma = w\frac{\partial}{\partial y} + w\frac{\partial}{\partial w} \tag{9.40}$$

which is, again, a second order vector field with respect to the alternative tangent bundle structure characterized by:

$$S' = \mathrm{d}y \otimes \frac{\partial}{\partial w} \qquad \Delta' = w\frac{\partial}{\partial w} \tag{9.41}$$

Remark 4 Postponing to a future work a carefully analysis of such a question, we would stress the fact that we have considered a generic vector field (not of second order with respect to S and Δ) and we have searched for a diffeomorphism which transforms such a vector field into a second order one with respect to a novel tangent bundle structure. On the other side another situation is possible, that is, the one in which the given vector field is made into a second order one by selecting an appropriate tangent bundle structure. Of course the two situations are strictly related.

9.4 Dynamical Systems and Geometrical Structures: Hamiltonian Picture

As said before, in the Hamiltonian formalism, the fundamental geometric structure is the Liouville 1-form, θ,[5] whose differential is the canonical symplectic form ω on the cotangent bundle $\mathbf{T}^*\mathcal{Q}$, that is, a closed, non-degenerate 2-form on $\mathbf{T}^*\mathcal{Q}$. Once we have ω and the Hamiltonian function $\mathscr{H}$, we may always write the equation

$$i_{X_{\mathscr{H}}}\,\omega \;=\; \mathrm{d}\mathscr{H}\,, \tag{9.42}$$

where $X_{\mathscr{H}}$ is a vector field on $\mathbf{T}^*\mathcal{Q}$. Unlike the Lagrangian setting, the 2-form ω is always nondegenerate, and thus the previous equation has a unique solution $X_{\mathscr{H}}$ which is called the Hamiltonian vector field associated with $\mathscr{H}$. It is immediate to check that $X_{\mathscr{H}}$ is such that $\mathcal{L}_{X_{\mathscr{H}}}\,\omega = 0$, and that, in a coordinates system $(\mathbf{q},\ \mathbf{p})$ adapted to the cotangent bundle structure of $\mathbf{T}^*\mathcal{Q}$, (9.42) "becomes" Hamilton equations:

$$\frac{d}{dt}q^i = \frac{\partial\mathscr{H}}{\partial p_i} = \{q^i,\ \mathscr{H}\} \qquad \frac{d}{dt}p_i = -\frac{\partial\mathscr{H}}{\partial q^i} = -\{p_i,\ \mathscr{H}\}\,. \tag{9.43}$$

Furthermore, it is important to note that ω is independent of the Hamiltonian function $\mathscr{H}$. It has a "kinematical" character, it is canonically defined on any cotangent bundle independently of any possible dynamics. This is clearly in contrast with what happens in the Lagrangian setting where the Lagrangian 2-form $\omega_{\mathscr{L}}$ always depends on the Lagrangian function $\mathscr{L}$. In some sense $\mathscr{L}$ has both "kinematical" and "dynamical" contents, while in the Hamiltonian picture the symplectic structure has a kind of "universal" character.

Since ω is a symplectic form, it is invertible, and its inverse is denoted by Λ. We recall that ω defines a base-invariant fiberwise isomorphism between $\mathbf{TT}^*\mathcal{Q}$ and $\mathbf{T}^*\mathbf{T}^*\mathcal{Q}$:

$$\omega^\flat \;\mid\; \mathbf{TT}^*\mathcal{Q} \to \mathbf{T}^*\mathbf{T}^*\mathcal{Q} \;\;:\;\; (\mathbf{q},\ \mathbf{X}) \mapsto (\mathbf{q},\ i_{\mathbf{X}}\omega) \tag{9.44}$$

then Λ is the inverse of this isomorphism. In a coordinates system $(\mathbf{q},\ \mathbf{p})$ adapted to the cotangent bundle structure of $\mathbf{T}^*\mathcal{Q}$, we have $\Lambda = \frac{\partial}{\partial q^i} \wedge \frac{\partial}{\partial p_i}$. The bivector field Λ allows us to define a POISSON BRACKET (see [11], Sect. 4.3.1) on smooth functions on $\mathbf{T}^*\mathcal{Q}$ in the following way:

$$\{f,\ g\} = \Lambda(df,\ dg) \;\;\forall f,\ g \in C^\infty(\mathbf{T}^*\mathcal{Q})\,. \tag{9.45}$$

Clearly, once we have Λ and $\mathscr{H}$ it is immediate to check that (9.42) may be alternatively written as

$$X_{\mathscr{H}} \;=\; i_{\mathrm{d}\mathscr{H}}\,\Lambda\,. \tag{9.46}$$

[5] $\theta = \gamma \circ T\pi$, where γ is a section of $\mathbf{T}^*\mathcal{Q}$ and π is the canonical projection of the cotangent bundle.

It is clear that in general one may use a bi-vector field Λ which is not invertible and previous equations would still make sense. Indeed, Hamilton equations may be formulated starting only with a Poisson Bracket, that is, a bivector field Λ satisfying $[\Lambda,\ \Lambda] = 0$, where $[\,\cdot\,,\,\cdot\,]$ denotes the Schouten–Nijenhuis bracket (see Appendix D in [11]). If Λ is the inverse of some symplectic form ω, then $[\Lambda,\ \Lambda] = 0$ is automatically satisfied, but not every Poisson tensor comes from a symplectic form. Indeed, it would be possible to have a Poisson bi-vector field which is not invertible, and thus, which is not the inverse of a symplectic form. This is the case, for example, of the canonical Poisson bi-vector field on the dual of the Lie algebra of a Lie group. As an example, consider the Lie algebra $\mathfrak{g}$ of a finite-dimensional Lie group G, and the dual $\mathfrak{g}^*$ of $\mathfrak{g}$. The elements in $\mathfrak{g}$ may be identified with the linear functions on the vector space $\mathfrak{g}^*$ by means of the map $a \mapsto f_a$ where a is in $\mathfrak{g}$ and f_a is the linear function on $\mathfrak{g}^*$ given by

$$f_a(\xi) \ = \ \xi(a) \tag{9.47}$$

for every $\xi \in \mathfrak{g}$. Since the differentials of the linear functions on the vector space $\mathfrak{g}^*$ generate the module of differential one-forms on $\mathfrak{g}^*$, we may define a bi-vector field Λ by

$$\Lambda(\mathrm{d}f_a,\ \mathrm{d}f_b) \ := f_{[a,\,b]}\,, \tag{9.48}$$

where $[\ ,\ ]$ denotes the Lie product in $\mathfrak{g}$, and extending Λ by linearity. Then, the fact that the bi-vector field Λ satisfies $[\Lambda,\ \Lambda] = 0$ essentially follows from the fact that $[\ ,\ ]$ satisfies the Jacobi identity (see [11, 21]). Furthermore, it is easy to see that Λ is in general not invertible (for instance when $\mathfrak{g}$ is the Lie algebra of the unitary group $\mathcal{U}(\mathcal{H})$ of some finite-dimensional complex Hilbert space $\mathcal{H}$).

Note that (9.42) is well-defined not only on the cotangent bundle $\mathbf{T}^*\mathcal{Q}$ of some configuration space $\mathcal{Q}$, but may be defined on any symplectic manifold in the sense that if $\mathcal{M}$ is any $2n$-dimensional smooth manifold endowed with a symplectic form ω, then, it always makes sense to define the Hamiltonian vector field associated with a given Hamiltonian function according to (9.42), for instance, on the 2-dimensional sphere. Furthermore, (9.46), as we have already remarked, makes sense in an even more general context because $\mathcal{M}$ needs not be even-dimensional in order for a Poisson bivector Λ to exists on it.

Now, let us consider a Hamiltonian vector field system with respect to the symplectic structure given by Ω. Let us consider a diffeomorphism $\phi \mid \mathcal{M} \to \mathcal{M}$. It is immediate to check that (9.42) changes equivariantly in the sense that $\phi^*\Omega$ is another symplectic form on $\mathcal{M}$, and $\phi^* X_{\mathscr{H}}$ is the Hamiltonian vector field associated with $\phi^*\mathscr{H}$ by means of $\phi^*\Omega$. If ϕ is a symmetry for our Hamiltonian vector field (that is, $\phi^* X_{\mathscr{H}} = X_{\mathscr{H}}$), then, we set $\Omega_\phi := \phi^*\Omega$, and we define the (1, 1) tensor field associated with ϕ and the initial symplectic form

$$T_\phi = \Lambda \circ \Omega_\phi\,. \tag{9.49}$$

Since Ω and Ω_ϕ are invariant with respect to $X_{\mathscr{H}}$, it follows that T_ϕ is also invariant. Then, according to [13] [Formula (2.4.12) at p. 170], it is possible to define the T-

differential, say d_T which acts on functions as $T \circ \mathrm{d}$. Now, given a smooth constant of the motion for our Hamiltonian field, that is, a smooth function f such that $\mathcal{L}_{X_{\mathscr{H}}} f = 0$, it is possible to define the following closed 2-form on $\mathcal{M}$

$$\omega_f = \mathrm{d}\mathrm{d}_T f \,. \tag{9.50}$$

It is immediate to check that ω_f is invariant with respect to $X_{\mathscr{H}}$, indeed

$$\begin{aligned} \mathcal{L}_{X_{\mathscr{H}}}\, \omega_f &= \mathcal{L}_{X_{\mathscr{H}}}\, (\mathrm{d}\mathrm{d}_T f) \;=\; \mathrm{d}\left(\mathcal{L}_{X_{\mathscr{H}}}\, (T \circ \mathrm{d} f)\right) \;= \\ &= \mathrm{d}\left(\left(\mathcal{L}_{X_{\mathscr{H}}}\, T\right) \circ \mathrm{d} f\right) + \mathrm{d}\left(T \circ \mathcal{L}_{X_{\mathscr{H}}}\, (\mathrm{d} f)\right) \;=\; 0\,. \end{aligned} \tag{9.51}$$

If ω_f is nondegenerate (i.e., symplectic), this is equivalent to $i_{X_{\mathscr{H}}}\, \omega_f$ being a non-zero closed 1-form. It may happen that $i_{X_{\mathscr{H}}}\, \omega_f$ is actually exact (for instance if $\mathcal{M}$ is contractible), in which case we obtain another Hamiltonian description of $X_{\mathscr{H}}$ with respect to another symplectic form and another Hamiltonian function. It is worth noting that this procedure may be iterated, that is, out of any constant of the motion one may construct an invariant 2-form which, if non-degenerate, is a new, alternative, symplectic form. Moreover, consider two of such symplectic forms, say ω_1 and ω_2, and consider the two associated Poisson bracket. If their sum is again a Poisson bracket, then the two symplectic structure are COMPATIBLE IN THE SENSE OF MAGRI[6] that is, the recursion operator $N = \omega_2^\sharp\, \omega_1^\flat$ may have n simple eigenvalues which may turn out to be n functionally independent constant of the motion in involution and thus, by ARNOLD- LIOUVILLE THEOREM, the Hamiltonian, with respect both the symplectic structures, field is also completely integrable.

To resume, starting with a symplectic structure, an Hamiltonian and a symmetry for the corresponding Hamiltonian vector field which is not a canonical symmetry, it is possible to construct, in principle, other symplectic forms that provide an alternative description of the same Hamiltonian field. Moreover, under suitable conditions, they are compatible in the sense of Magri and thus guarantee the complete integrability of the Hamiltonian system (see also [22]).

9.5 Dynamical Systems and Geometrical Structures: Quantum Systems

The existence of alternative symplectic structures invariant under the infinitesimal action of a dynamical vector field allows for the existence of alternative quantum descriptions as it may be shown by means of the Weyl formalism. The subject of this section is to briefly review how these alternative quantum descriptions arise. For this purpose, we need to recall what WEYL SYSTEMS are. Let us consider a symplectic vector space $(\mathbb{V},\ \omega)$, and a complex, separable Hilbert space say $\mathcal{H}$. A WEYL SYSTEM

[6] See [22].

is a map from $\mathbb{V}$ to the group $\mathcal{U}(\mathcal{H})$ of unitary operators over $\mathcal{H}$

$$W \mid \mathbb{V} \to \mathcal{U}(\mathcal{H}) \ : \ z \mapsto W(z) \tag{9.52}$$

such that

$$W(z + z') = W(z)W(z')\, e^{-\frac{i}{2\hbar}\omega(z,\, z')}\,, \tag{9.53}$$

so that

$$W(z)W(z') = W(z')W(z)\, e^{\frac{i}{\hbar}\omega(z,\, z)}\,, \tag{9.54}$$

which means that the operators associated with elements in the same Lagrangian subspace[7] of $(\mathbb{V},\ \omega)$ commute. Furthermore, W is required to be STRONGLY CONTINUOUS, that is, it must hold that

$$lim_{z \to z_0}\, ||W(z) - W(z_0)||_{sup} = 0 \tag{9.55}$$

where $||\ \cdot\ ||_{sup}$ is the *sup* norm on the Banach space of linear operators over $\mathcal{H}$, $\mathcal{OP}(\mathcal{H})$.

From (9.53), it follows that when z and z' are in the same one-dimensional subspace of $\mathbb{V}$, that is, $z' = az$ for some $a \in \mathbb{R}$, then:

$$W(z + z') = W(z)\, W(z')\,, \tag{9.56}$$

that is, $W(az)$ is a one-parameter group of unitary operators labelled by the parameter $a \in \mathbb{R}$. Being W strongly continuous, the STONE- VON NEUMANN THEOREM implies that

$$W(az) = e^{ia\, G(z)} \tag{9.57}$$

for some (possibly unbounded) self-adjoint operator G. Thus, (9.54) may be written as

$$e^{i\, G(z)} e^{i\, G(z')}\, e^{-i\, G(z)} e^{-i\, G(z')} = e^{\frac{i}{\hbar}\, \omega(z,\, z')}\,, \tag{9.58}$$

from which we recognize WEYL COMMUTATION RELATIONS. If $\{\phi_t\}_{t \in \mathbb{R}}$ is a one-parameter group of symplectomorphisms, then we can define:

$$W_t\,(z) =: \mathcal{W}\,(\phi_t(z))\,. \tag{9.59}$$

This is a one parameter group of unitary transformations which may be represented as a similarity transformation by means of a one-parameter group of automorphisms on the space of operators, namely $\{\phi_t\}$:

$$W_t\,(z) = e^{it\widehat{H}}\ W\ (z)\ e^{-it\widehat{H}}\,, \tag{9.60}$$

[7] We recall that given a symplectic vector space, say $(\mathbb{V},\ \omega)$, a Lagrangian subspace of $\mathbb{V}$ with respect to the symplectic structure ω, say $\mathbb{L}$, is a subspace $\mathbb{L} = \{z \in \mathbb{V} \ : \ \omega(z_i,\, z_j) = 0\ \ \forall z_i,\, z_j \in \mathbb{L}\}$.

where $\widehat{H}$ is the infinitesimal generator derived by Stone-Von Neumann theorem. In some cases, ϕ_t may arise as the flow associated with the dynamical evolution generated by a linear vector field Γ on $\mathbb{V}$.

At this point, it is impossible not to recall von Neumann's theorem. This theorem states that Weyl systems do exist for any finite-dimensional symplectic vector space $\mathbb{V}$, and provide an explicit realization for both W and the Hilbert space $\mathcal{H}$. Specifically, $\mathbb{V}$ is decomposed (in a not unique way) into the direct sum of Lagrangian subspaces,[8] $\mathbb{V} = \mathbb{L}_1 \oplus \mathbb{L}_2$, and we define $U =: W|_{\mathbb{L}_2}$ and $V =: W|_{\mathbb{L}_1}$. Then, the Hilbert space $\mathcal{H}$ is realized as the space $\mathcal{H} = L^2(L, d^n x)$ of square-integrable complex functions with respect to the translationally-invariant Lebesgue measure on the Lagrangian subspace $\mathbb{L}_1$. Finally, the Weyl system is realized as follows:

$$\begin{aligned} (V(z_1)\,\psi)(x) &= \psi(x + z_1) \\ (U(z_2)\,\psi)(x) &= e^{i\,\omega(x,z_2)}\psi(x)\ . \end{aligned} \tag{9.61}$$

where $z_1, x \in \mathbb{L}_1$ and $z_2 \in \mathbb{L}_2$. Setting $z_1 \equiv q$ and $z_2 \equiv p$, the infinitesimal generators of $U(z_1)$ and $V(z_2)$ are:

$$\begin{aligned} V(z_1) &= e^{iq^j P_j} \;\rightarrow\; \left(P_j\,\psi\right)(\mathbf{x}) = i\frac{d}{dx^j}\psi(\mathbf{x}) \\ U(z_2) &= e^{ip_j Q^j} \;\rightarrow\; \left(Q^j\,\psi\right)(\mathbf{x}) = q^j\psi(\mathbf{x})\,. \end{aligned} \tag{9.62}$$

The definition of Weyl system, as well as its explicit realization given by von Neumann's theorem, depends on both the linear structure and the symplectic form ω on $\mathbb{V}$. Specifically, von Neumann's theorem states that the realizations of a Weyl system on the Hilbert spaces of square-integrable functions on different Lagrangian subspaces of the same symplectic vector space are unitarily related. This means that every invertible smooth map ϕ from $\mathbb{V}$ to itself such that it preserves the given linear structure and symplectic bilinear form ω on $\mathbb{V}$, will give rise to a unitary transformation between the von Neumann realization of $(\mathbb{V}, \omega)$ on the space of square-integrable functions on the Lagrangian subspace L with respect to the Lebesgue measure on it, and the von Neumann realization of $(\mathbb{V}, \omega)$ on the space of square-integrable functions on the Lagrangian subspace $\phi(L)$ with respect to the Lebesgue measure on it.

This result clearly depends on the fact that we fix the linear structure as well as the symplectic form on $\mathbb{V}$. Consequently, if alternative linear structures and alternative symplectic forms are given on the same set $\mathbb{V}$, we obtain alternative Weyl systems as well as alternative realizations of Weyl systems in terms of the von Neumann theorem. This instance is thoroughly investigated in [23], and will be briefly recalled here by means of a concrete example.

[8] Given an even dimensional symplectic vector space, such a decomposition is always possible ([11], Sect. 5.2.2).

Consider a symplectic vector space $(\mathbb{V},\, \omega)$, where $\mathbb{V} = \mathbb{R}^2$ with the standard vector space structure, and let (q, p) be Cartesian coordinates adapted to the linear structure of $\mathbb{V}$ in which ω takes its canonical form. Next, consider the nonlinear diffeomorphism ϕ of $\mathbb{V}$ to itself given by:

$$(Q,\, P) \,\equiv\, \phi(q, p) \,:=\, (q\, K(|q|),\, p)\,, \tag{9.63}$$

where K is a smooth function, such that $K(|q|) + q\frac{\partial K(|q|)}{\partial q} \neq 0$, in order for this to represent a diffeomorphism. We may use (Q, P) as Cartesian coordinates adapted to a new linear structure on $\mathbb{V} = \mathbb{R}^2$ given by the addition operation $(Q, P) + (Q', P') = (Q + Q', P + P')$ and the scalar multiplication operation $a \cdot (Q, P) = (aQ, aP)$ with $a \in \mathbb{R}$. This new vector space will be denoted by $\mathbb{V}_\phi$. Note that the vector space structure on $\mathbb{V}_\phi$ may be described in the old vector space $\mathbb{V}$ by the following addition and scalar multiplication operations expressed in the old coordinates:

$$(q,\, p) \,+_\phi\, (q',\, p') \,:=\, \phi^{-1}(\phi(q,\, p) \,+\, \phi(q',\, p')) \tag{9.64}$$

$$a \,\cdot_\phi\, (q,\, p) \,:=\, \phi^{-1}(a \,\cdot\, \phi(q,\, p))\,, \tag{9.65}$$

where $+$ and $\cdot$ are the addition and scalar multiplication operations on $\mathbb{V}_\phi$. Then, we may take ω_ϕ to be the symplectic bilinear form on $\mathbb{V}_\phi$ which takes its canonical form with respect to (Q, P) and define the symplectic vector space $(\mathbb{V}_\phi,\, \omega_\phi)$. Note that the symplectic vector spaces $(\mathbb{V},\, \omega)$ and $(\mathbb{V}_\phi,\, \omega_\phi)$ are nonlinearly related by means of ϕ.

Now, we build the Weyl system associated with $(\mathbb{V},\, \omega)$ by selecting the Lagrangian subspace $\mathcal{L} \,=\, \text{span}\{\,(q,\, 0)\,\}$ endowed with the Lebesgue measure $\mathrm{d}\mu = \mathrm{d}q$, so that the Hilbert space of the von Neumann representation is $\mathfrak{L}^2(\mathcal{L},\, \mathrm{d}q)$. The operators U and V are then defined by:

$$\begin{aligned} (U(\alpha)\psi)(x) \,&=\, e^{i\alpha q}\psi(x) \\ (V(\beta)\psi)(x) \,&=\, \psi(x \,+\, \beta) \end{aligned} \tag{9.66}$$

whose generators turn to be $\hat{x} \,=\, q$ and $\hat{\pi} \,=\, -i\frac{\partial}{\partial q}$ which satisfy the canonical commutation relations on the Hilbert space $\mathfrak{L}^2(\mathcal{L},\, \mathrm{d}q)$. From these generators we may build the creation and annihilation operators $\hat{a}^\dagger \,=\, \frac{\hat{x} - i\hat{\pi}}{\sqrt{2}}$ and $\hat{a} \,=\, \frac{\hat{x} + i\hat{\pi}}{\sqrt{2}}$, so that the Hilbert space $\mathfrak{L}^2(\mathcal{L},\, \mathrm{d}q)$ "arises" as the Fock space generated by:

$$|n\rangle \,=\, \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n\,|0\rangle \tag{9.67}$$

with $n = 0, 1, 2, \ldots, n, \ldots$ and where $|0\rangle$ is the vacuum state annihilated by $\hat{a}$.

Similarly, we build the Weyl system associated with $(\mathbb{V}_\phi,\, \omega_\phi)$ by selecting the Lagrangian subspace $\mathcal{L}' \,=\, \text{span}\{\,(Q,\, 0)\,\}$ endowed with the Lebesgue measure $\mathrm{d}\mu = \mathrm{d}Q$, so that the Hilbert space is $\mathfrak{L}^2(\mathcal{L}',\, \mathrm{d}Q)$ and the operators U' and V'

are given by:

$$\begin{aligned}(U'(\alpha)\psi)(x') &= e^{i\alpha Q}\psi(x') \\ (V'(\beta)\psi)(x') &= \psi(x' + \beta)\end{aligned} \tag{9.68}$$

whose generators turn to be $\hat{x}' = Q$ and $\hat{\pi}' = -i\frac{\partial}{\partial Q}$ with canonical commutation relations on the Hilbert space $\mathfrak{L}^2(\mathcal{L}', \mathrm{d}Q)$. Again, we may build creation and annihilation operators $\hat{A}^\dagger = \frac{\hat{x}' - i\hat{\pi}'}{\sqrt{2}}$ and $\hat{A} = \frac{\hat{x}' + i\hat{\pi}'}{\sqrt{2}}$, so that the Hilbert space $\mathfrak{L}^2(\mathcal{L}', \mathrm{d}Q)$ "arises" as the Fock space generated by:

$$|N\rangle = \frac{1}{\sqrt{N!}}(\hat{A}^\dagger)^n |0_\phi\rangle \tag{9.69}$$

with $N = 0, 1, 2, \ldots, n, \ldots$ and where $|0_\phi\rangle$ is the vacuum state annihilated by $\hat{A}$. Note that we may realize the operator $V'(\beta)$ on the Hilbert space $\mathfrak{L}^2(\mathcal{L}, \mathrm{d}q)$ where it implements translations with respect to the addition operation $+_\phi$:

$$(V'(\beta)\psi)(x) = \psi(x +_\phi \beta)\,. \tag{9.70}$$

Now, we note that the Lagrangian subspaces $\mathcal{L}$ and $\mathcal{L}'$ coincide because they are the subspaces characterized by $p = P = 0$. However, since the linear structure on $\mathbb{V}$ is nonlinearly related with the linear structure on $\mathbb{V}_\phi$, it follows that the Lebesgue measures on $\mathcal{L}$ and $\mathcal{L}'$ are no longer linearly related, and thus square integrable functions with respect to one measure need not be square integrable with respect to the other. In particular, we may obviously look at $\hat{x}$ and $\hat{\pi}$ as linear operators on both $\mathfrak{L}^2(\mathcal{L}, \mathrm{d}q)$ and $\mathfrak{L}^2(\mathcal{L}', \mathrm{d}Q)$ because $\mathcal{L}$ and $\mathcal{L}'$ are the same subsets of $\mathbb{R}^2$, however, it turns out that $\hat{x}$ is self-adjoint on both the Hilbert spaces, while $\hat{\pi}$ is self-adjoint only on $\mathfrak{L}^2(\mathcal{L}, \mathrm{d}q)$. Consequently, the algebra "generated" by the operators $\hat{x}$, $\hat{\pi}$, $\mathbb{I}$ together with their adjoints on $\mathfrak{L}^2(\mathcal{L}, \mathrm{d}q)$ is actually a C^*-algebras, while that generated by $\hat{x}$, $\hat{\pi}$, $\mathbb{I}$ together with their adjoints on $\mathfrak{L}^2(\mathcal{L}', \mathrm{d}Q)$ is not (see [23] for more details). From this discussion, it should be clear that, in the construction of Weyl systems and their associated von Neumann realizations, it should be explicitly stated the relevant assumption regarding the existence of a specific (and fixed) symplectic vector space structure on $\mathbb{V}$. Furthermore, it should be clear that, whenever alternative symplectic vector space structures are available at the same time, we may face a particularly rich situation in which nonlinearly related formulations of quantum mechanics are possible.

9.6 Conclusions

The description of a physical system by means of a vector field Γ on some carrier manifold $\mathcal{M}$ is something which we should arrive at, rather than to start with. Experimental data provide us with trajectories on some configuration space, and it is part

of the job of a theoretician to extract a differential equation out of them. As we have argued in Sect. 9.2, in general it is possible to pass from the experimental trajectories to an implicit differential equation. This is a subset (hopefully a submanifold) of some carrier space $\mathcal{M}$ which has to be built out of the experimental data. In this case, obtaining a solution to the inverse problem of the dynamics, that is, finding a Lagrangian or Hamiltonian description of the given physical system, is particularly difficult. Some comments on this situation are given in Appendix. However, in some cases it is possible to pass from the experimental trajectories to an explicit differential equations the solutions of which are (appropriate lifts of) the trajectories we started with, and we obtain a vector field Γ on the carrier manifold $\mathcal{M}$.

After explaining the main points necessary to the construction of Γ from experimental trajectories, we passed, in Sects. 9.3 and 9.4, to analyse the process of "tensorialization" of the Lagrangian and Hamiltonian description of the physical systems associated with Γ. In this way, it is possible to single out the qualitative features that characterize a given picture of Classical Mechanics, and the possibility of obtaining alternative Lagrangian or Hamiltonian descriptions for the same physical systems is clearly enlightened. In the Lagrangian picture, the carrier manifold $\mathcal{M}$ turns out to be diffeomorphic to the tangent bundle $\mathbf{T}Q$ of the configuration space Q, and, once the tangent bundle structure is fixed, alternative Lagrangian descriptions are usually obtained by means of the construction (if possible) of alternative Lagrangian functions for the same vector field Γ on $\mathcal{M} \cong TQ$ [13]. However, once the tangent bundle structure of $\mathcal{M}$ is "tensorialized" in the couple $(S,\ \Delta)$ as it is recalled in Sect. 9.3, we pointed out that it is also possible to change the tangent bundle structure of $\mathcal{M}$ so that the same vector field Γ becomes a second order vector field for an alternative tangent bundle structure, and thus the possibility of a Lagrangian description of Γ with respect to this alternative tangent bundle structure has to be investigated. This instance can also be read from the opposite point of view. Specifically, we may look for a tangent bundle structure on $\mathcal{M}$ (if possible) in which Γ is a second order vector field admitting of a Lagrangian description. Furthermore, in some cases it could be necessary to reparametrize Γ in such a way that it becomes a complete vector field (e.g., the Kepler problem), and this reparametrization would in general make the reparametrized vector field no longer second order with respect to the "old" tangent bundle structure so that a Lagrangian description for the reparametrized vector field is not possible. However, we may ask if there is an alternative tangent bundle structure on $\mathcal{M}$ with respect to which the reparametrized vector field is a second order vector field so that search for a Lagrangian description for the reparametrized vector field in the "new" tangent bundle structure is meaningful. At the end of Sect. 9.3 we provided some simple examples where this program can be successfully followed, and we plan to take on a more systematic analysis of this instance in future works.

In Sect. 9.4, we applied the "tensorialization" process to the Hamiltonian picture of dynamics. In this case, we showed how the diffeomorphism invariance of the tensorial description allows us to obtain alternative Hamiltonian descriptions associated with symmetries and constants of the motion. Specifically, let Γ be the dynamical vector field , which is assumed to be the Hamiltonian vector field of some Hamiltonian function $\mathscr{H}$ with respect to the symplectic form ω. If $\phi\colon \mathcal{M} \to \mathcal{M}$ is

a diffeomorphism which is a symmetry for the dynamics ($\phi^*\Gamma = \Gamma$), we may form the symplectic form $\omega_\phi = \phi^*\omega$ and the $(1-1)$ tensor field $T_\phi = \Lambda \circ \omega_\phi$. Clearly, both ω_ϕ and T_ϕ are invariant with respect to Γ. Then, if f is a constant of the motion for the dynamics ($\Gamma(f) = 0$), we have that $\omega_f = \mathrm{d}\,\mathrm{d}_{T_\phi} f = \mathrm{d}\,T_\phi(\mathrm{d}f)$ is a two-form which is invariant with respect to the dynamical vector field Γ. When ω_f is non-degenerate, it provides us with an alternative Hamiltonian description for Γ as the locally Hamiltonian vector field for the closed one-form $i_\Gamma \omega_f$.

In Sect. 9.5, we recalled the deep connection between alternative symplectic vector space structures and alternative Weyl systems leading to alternative quantum descriptions and alternative commutation relations. Indeed, a Weyl system is a map from a symplectic vector space $(\mathbb{V}, \omega)$ to the group of unitary operators on some Hilbert space satisfying additional properties (see Sect. 9.5 for details). Consequently, the existence of alternative linear structures and alternative symplectic structures on $\mathbb{V}$ gives rise to an alternative structure of symplectic vector space on $\mathbb{V}$ and to an alternative realization of the Weyl system by means of von Neumann's theorem. According to the discussion in Sect. 9.4, alternative symplectic structures may be "dynamically" obtained starting with a (linear) vector field on $\mathbb{V}$ thus showing how to pass from classical-like trajectories to the quantum commutation relations encoded in the infinitesimal generators of the Weyl system. Furthermore, the coexistence of nonlinearly related alternative symplectic vector space structures implies the coexistence of nonlinearly related alternative formulations of quantum mechanics, together with the coexistence of nonlinearly related alternative procedures of second quantization [24].

Appendix: Inverse Problem for Implicit Differential Equations

In Sect. 9.2 we saw how, in general, experimental data lead the theoretician to build a submanifold of $\mathbf{TTQ}$, that is, an implicit differential equation on (a submanifold of) the tangent bundle $\mathbf{TQ}$. Within this context the inverse problem is much more complicated to address than it is in the explicit case. Essentially, this is due to the fact that the *Euler-Lagrange equations* are formulated by means of an implicit differential equation on $\mathbf{T}^*\boldsymbol{Q}$ rather than by means of an implicit differential equation on $\mathbf{TQ}$, even though the Lagrangian function is defined on the tangent bundle $\mathbf{TQ}$. Indeed, given the Lagrangian function $\mathscr{L}$, we have $\mathrm{d}\mathscr{L}\colon \mathbf{TQ} \to \mathbf{T}^*\mathbf{TQ}$, and thus $\mathrm{d}\mathscr{L}(\mathbf{TQ})$ is a submanifold of $\mathbf{T}^*\mathbf{TQ}$. By means of the inverse of the canonical Tulczyjew isomorphism $\tau\colon \mathbf{TT}^*\boldsymbol{Q} \to \mathbf{T}^*\mathbf{TQ}$ [25], we obtain a submanifold of $\mathbf{TT}^*\boldsymbol{Q}$, i.e., an implicit differential equation on $\mathbf{T}^*\boldsymbol{Q}$. Explicitly, we have

$$\mathrm{d}\mathscr{L} \;\mid\; \mathbf{TQ} \to \mathbf{T}^*\mathbf{TQ} \;:\; (q^i,\, v^i) \mapsto \left(q^i,\, v^i,\, \frac{\partial \mathscr{L}}{\partial q^i},\, \frac{\partial \mathscr{L}}{\partial v^i}\right), \tag{9.71}$$

while the Tulczyjew isomorphism between $\mathbf{TT}^*Q$ and $\mathbf{T}^*\mathbf{T}Q$ is defined by

$$\tau \;|\; \mathbf{TT}^*Q \to \mathbf{T}^*\mathbf{T}Q \;:\; (q^i,\, p_i,\, v_q^i,\, v_{p_i}) \mapsto (q^i,\, v_q^i,\, v_{p_i},\, p_i) \tag{9.72}$$

(see [25], Sect. 3). This is, in fact, a SYMPLECTOMORPHISM mapping the canonical symplectic form over $\mathbf{T}^*\mathbf{T}Q$, i.e., $\mathrm{d}q^i \wedge \mathrm{d}p_{q_i} + \mathrm{d}v^i \wedge \mathrm{d}p_{v_i}$, into the canonical symplectic form over $\mathbf{TT}^*Q$, i. e., $\mathrm{d}v_q^i \wedge \mathrm{d}p_{v_i} + \mathrm{d}q^i \wedge \mathrm{d}p_{q_i}$. By composing $\mathrm{d}\mathscr{L}$ and τ^{-1} we obtain a submanifold of $\mathbf{T}^*\mathbf{T}Q$, say Σ, given by

$$\Sigma := \left(\tau^{-1} \circ \mathrm{d}\mathscr{L}\right)(\mathbf{T}Q) = \left\{ (q^i, p_i,\, v_q{}^i,\, v_{p_i}) \in \mathbf{TT}^*Q \mid p_i = \frac{\partial \mathscr{L}}{\partial v^i}\,,\; v_{p_i} = \frac{\partial \mathscr{L}}{\partial q^i} \right\}. \tag{9.73}$$

Writing i_Σ for the canonical immersion of Σ into $\mathbf{TT}^*Q$, it follows that Σ is a Lagrangian (or simply isotropic if L is not regular) submanifold of $\mathbf{TT}^*Q$ because

$$i_\Sigma^* \left(\mathrm{d}v_q^i \wedge \mathrm{d}p_{v_i} + \mathrm{d}q^i \wedge \mathrm{d}p_{q_i} \right) = \mathrm{d}v_q^i \wedge \mathrm{d}\left(\frac{\partial \mathscr{L}}{\partial v^i} \right) + \mathrm{d}q^i \wedge \mathrm{d}\left(\frac{\partial \mathscr{L}}{\partial q^i} \right) = 0 \tag{9.74}$$

since $\mathscr{L}$ depends only on $(q^i,\, v_q{}^i)$. Note that, with the prescription that $v_{p_i} = \frac{d}{dt} p_i$, it immediately follows that Σ as defined in (9.73) is the submanifold of $\mathbf{TT}^*Q$ on which the EULER- LAGRANGE EQUATIONS

$$\frac{d}{dt} \frac{\partial \mathscr{L}}{\partial v^i} = \frac{\partial \mathscr{L}}{\partial q^i} \tag{9.75}$$

are identically satisfied.

Remark 5 A similar construction is possible for the Hamiltonian case where it clearly emerges that the submanifold of $\mathbf{TT}^*Q$ one obtains is the graph of a vector field, that is, the equations are always explicit ones. Consider the cotangent bundle $\mathbf{T}^*Q$ of the configuration space Q and a Hamiltonian function $\mathscr{H} \;|\; \mathbf{T}^*Q \to \mathbb{R}$. Via its differential

$$\mathrm{d}\mathscr{H} \;|\; \mathbf{T}^*Q \to \mathbf{T}^*\mathbf{T}^*Q\,, \tag{9.76}$$

we can define a submanifold Σ of $\mathbf{T}^*\mathbf{T}^*Q$ by setting $\Sigma := \mathrm{d}\mathscr{H}(\mathbf{T}^*Q)$. Differently from the Lagrangian case, we have that $\mathbf{T}^*\mathbf{T}^*Q$ is isomorphic to $\mathbf{TT}^*Q$ because the Poisson structure Λ associated with the canonical symplectic structure over $\mathbf{T}^*Q$ define an isomorphism between differential forms and vector fields on $\mathbf{T}^*Q$. With an evident abuse of notation, we denote this isomorphism with Λ. By means of Λ, we obtain the implicit differential equation $\Lambda(\Sigma)$ on $\mathbf{TT}^*Q$. Denoting by $X_{\mathscr{H}}$ the Hamiltonian vector field associated with $\mathscr{H}$ by means of the Poisson tensor Λ, that is, $X_{\mathscr{H}} = \Lambda(\mathrm{d}\mathscr{H})$, the following diagram may be defined:

$$\begin{array}{ccc} \mathbf{TT}^*Q & \xleftarrow{\quad\Lambda\quad} & \mathbf{T}^*\mathbf{T}^*Q \\ & {\scriptstyle X_{\mathscr{H}}}\nwarrow \quad \nearrow{\scriptstyle \mathrm{d}\mathscr{H}} & \\ & \mathbf{T}^*Q\,, & \end{array} \tag{9.77}$$

and it follows that $\Lambda(\Sigma)$ is precisely $X_{\mathscr{H}}(\mathbf{T}^*Q)$. Consequently, being $\Lambda(\Sigma)$ the image of $\mathbf{T}^*Q$ through a vector field, it emerges that the dynamics is always an explicit one in the Hamiltonian case, as it is also clear from the standard form of the Hamilton equations.

We can say that EULER- LAGRANGE EQUATIONS force us to work with a Lagrangian submanifold of $\mathbf{TT}^*Q$, while, on the one hand, we saw in Sect. 9.2 how experimental data would naturally lead us to build a submanifold of $\mathbf{TT}Q$. Consequently, the following question is unavoidable: *how can these two seemingly uncompatible instances be related?* The essential difficulty is due to the absence of a natural, "pre-existing", symplectic structure on $\mathbf{TT}Q$. To be able to formulate the inverse problem for the submanifold of $\mathbf{TT}Q$ we construct out of the trajectories on Q, we would need a map:

$$\phi \;:\; \mathbf{T}Q \to \mathbf{T}^*Q \tag{9.78}$$

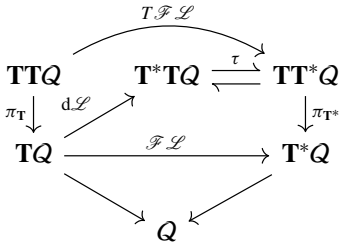
so that we would be able to map the submanifold of $\mathbf{TT}Q$, that we constructed out of trajectories, onto a submanifold of $\mathbf{TT}^*Q$ by means of the tangent map $T\phi$:

$$\begin{array}{ccc} \mathbf{TT}Q & \xrightarrow{\quad T\phi\quad} & \mathbf{TT}^*Q \\ {\scriptstyle \pi_{\mathbf{T}}}\downarrow & & \downarrow{\scriptstyle \pi_{\mathbf{T}^*}} \\ \mathbf{T}Q & \xrightarrow{\quad\phi\quad} & \mathbf{T}^*Q \\ & {\scriptstyle}\searrow \quad \swarrow{\scriptstyle} & \\ & Q & \end{array} \tag{9.79}$$

It may happen that the Lagrangian function itself could provide us with the map ϕ by means of the FIBER DERIVATIVE

$$\mathscr{F}\mathscr{L} \mid \mathbf{T}Q \to \mathbf{T}^*Q \;:\; (q^i,\, v^i) \mapsto \pi_{\mathbf{T}^*} \circ \tau \circ \mathrm{d}\mathscr{L} = \left(q^i,\, \frac{\partial \mathscr{L}}{\partial v^i}\right). \tag{9.80}$$

This map coincides with the map defined by the following diagram:



(9.81)

By means of the fiber derivative, the canonical symplectic structure $\Omega = \mathrm{d}p_i \wedge \mathrm{d}q^i$ and its potential $\theta = p_i \mathrm{d}q^i$ on $\mathbf{T}^*\boldsymbol{Q}$ can be pulled-back on $\mathbf{T}\boldsymbol{Q}$ to obtain

$$\begin{aligned} \theta_{\mathscr{L}} &= (\mathscr{F}\mathscr{L})^*\theta = \partial_i^v \mathscr{L} \mathrm{d}q^i \\ \Omega_{\mathscr{L}} &= (\mathscr{F}\mathscr{L})^*\Omega = \frac{\partial^2 \mathscr{L}}{\partial q^i \partial v^j} \mathrm{d}q^i \wedge \mathrm{d}q^j + \frac{\partial^2 \mathscr{L}}{\partial v^i \partial v^j} \mathrm{d}v^i \wedge \mathrm{d}q^j \,. \end{aligned} \tag{9.82}$$

By means of its tangent map, $T\mathscr{F}\mathscr{L}$, the symplectic structure on $\mathbf{TT}^*\boldsymbol{Q}$ and its potential, $\dot{\Omega}$ and $\dot{\theta}$, can be pulled-back on $\mathbf{TT}\boldsymbol{Q}$:

$$\begin{aligned} \dot{\theta}_{\mathscr{L}} &= (T\mathscr{F}\mathscr{L})^*\dot{\theta} \\ \dot{\Omega}_{\mathscr{L}} &= (T\mathscr{F}\mathscr{L})^*\dot{\Omega} \,. \end{aligned} \tag{9.83}$$

Note that, in general, $\Omega_{\mathscr{L}}$ and $\dot{\Omega}_{\mathscr{L}}$ are no longer symplectic form because they may present a kernel which depends on $\mathscr{L}$.

In conclusion, the Lagrangian plays a double role within the formulation of the inverse problem for implicit differential equations. First, it defines a Lagrangian submanifold Σ of $\mathbf{TT}^*\boldsymbol{Q}$, which represents the Lagrangian formulation of the dynamics. Second, it allows for the definition of a fiber derivative $\mathscr{F}\mathscr{L}$ which, if suitable regularity conditions on $\mathscr{L}$ are satisfied, would make it possible to impose that the pre-image of Σ through $T\mathscr{F}\mathscr{L}$ coincide with the submanifold of $\mathbf{TT}\boldsymbol{Q}$ on which the experimental data naturally live. See also Sect. 2.1 in [17] for another discussion about the inverse problem for implicit differential equations.

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Chapter 10
On the Thermodynamics of Supersymmetric Haldane–Shastry Spin Chains

F. Finkel, A. González-López, I. León and M. A. Rodríguez

Abstract In this short report we present some recent results on the thermodynamics of su($m|n$) supersymmetric spin chains of Haldane–Shastry type, with long-range position-dependent interactions. We first evaluate their partition function, and then show how to express it in terms of supersymmetric Haldane motifs. This key step makes it possible to derive the thermodynamic functions of the system in closed form through a modification of the usual transfer matrix approach. In particular, from the low-temperature behavior of the free energy we obtain a full description of the critical behavior of these chains for low values of m and n.

10.1 Introduction

The construction and study of simple models of complex physical systems often gives valuable insights on their characteristic properties. Thus, in condensed matter physics, magnetism and other related fields, spin chains have been a crucial ingredient of many theories capturing the key physical properties of complex phenomena. In particular integrable spin chains, which allow a complete description of the spectrum in closed form, have played an important role in this respect, even when they are sub-

Dedicated to our friend and colleague, Alberto Ibort, on his 60th anniversary.

Supported by MINECO (Spain) under grant FIS2015-63966-P.

F. Finkel · A. González-López · I. León · M. A. Rodríguez (✉)
Departamento de Física Teórica, Universidad Complutense de Madrid, 28040 Madrid, Spain
e-mail: rodrigue@ucm.es

F. Finkel
e-mail: ffinkel@ucm.es

A. González-López
e-mail: artemio@ucm.es

I. León
e-mail: ivleon@ucm.es

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_10

stantially simplified versions of the real systems they model. A paradigmatic example of this assertion is provided by the spin chain independently introduced by Haldane [25] and Shastry [33], which can be solved [18] by exploiting its connection to the integrable dynamical spin Sutherland model [24] using the so called Polychronakos freezing trick [31]. This model is of fundamental importance in condensed matter physics, since it is the simplest example of a system featuring fractional statistics [2, 13, 22, 23, 26, 28], and is also closely related to the one-dimensional Hubbard model of high-temperature superconductivity.

The Haldane–Shastry (HS) spin chain consists of N spins on fixed equispaced positions in a circular lattice, with long-range two-body interactions inversely proportional to the (chord) distance between the spins. This model has been extensively generalized in several substantially different directions without losing its integrability properties, which essentially stem from an underlying Yangian symmetry [11]. In the first place, while the original HS chain is closely related to the simple Lie algebra A_{N-1} (since the interaction depends only on the differences between the site coordinates), analogous models related to other simple algebras like BC_N, B_N, D_N, etc., have also been considered (see, e.g., [3–5, 17]). Secondly, the two-body interaction between the spins can in general be an elliptic Weierstrass-$\wp$ function of their distance, including as important degenerate cases rational, trigonometric or hyperbolic functions. Finally, although the original HS chain featured spin $1/2$ particles, the extensions of HS-type chains to su(m) and supersymmetric (su($m|n$)) spin have also been successfully achieved (see, e.g., [6, 7, 9, 27, 29]). In this work we shall be mainly concerned with the supersymmetric versions of the three families of spin chains of HS type with rational, trigonometric and hyperbolic interaction potentials related to the A_{N-1} algebra, respectively referred to as the Polychronakos–Frahm (PF) [20, 32], Haldane–Shastry and Frahm–Inozemtsev [21] (FI) chains.

The aim of this research is twofold. First of all, we shall compute the partition function of supersymmetric spin chains of HS type by taking advantage of their connection with supersymmetric dynamical spin Calogero–Sutherland models. We will then show that this partition function coincides with that of a suitable inhomogeneous vertex model, whose spectrum can be described using the supersymmetric version of Haldane's motifs. Using the latter description we shall achieve our second main goal, namely that of computing in closed form the free energy per site (and, hence, other thermodynamic functions of interest like the magnetization, densities, etc.) in the thermodynamic limit. By analyzing the asymptotic behavior of the free energy at low temperatures and comparing it to that of a $1+1$ dimensional conformal field theory (CFT) [1, 12], we shall be able to determine the critical behavior of the models under study as a function of the chemical potentials of each species. In particular, we shall compute the value of the central charge of the corresponding CFT in each of the critical regions in chemical potential space.

We shall end by outlining the organization of this report. Section 10.2 contains some basic facts, setting the notation and defining the models under consideration. In Sect. 10.3 we will evaluate their partition functions in closed form, while Sect. 10.4 is devoted to the computation of the free energy per site in the thermodynamic limit.

The asymptotic behavior of the free energy at low temperature is derived in Sect. 10.5, and it is then applied to the analysis of the criticality properties of the su(1|1) models. Finally, we present our conclusions and some comments on future work in Sect. 10.6.

10.2 Preliminaries

We introduce in this section the models under consideration and the notation and main ingredients of the theory. The model we shall be interested in is a supersymmetric su($m|n$) spin chain, that is, a one-dimensional lattice each of whose N sites is occupied by a particle with m bosonic and n fermionic degrees of freedom. The states of this system belong to the Hilbert space $\Sigma^{(m|n)} = \otimes_{i=1}^{N} \mathbf{C}^{m+n}$ with basis:

$$|\mathbf{s}\rangle = |s_1 \dots s_N\rangle = |s_1\rangle \otimes \cdots \otimes |s_N\rangle, \quad s_i \in \{1, \dots, m+n\} \tag{10.1}$$

The supersymmetric character of the chain is introduced by considering the state $|s_i\rangle$ as bosonic if $s_i \in \{1, \dots, m\}$ or fermionic if $s_i \in \{m+1, \dots, m+n\}$. The exchange operator, $P_{ij}^{(m|n)}$ (with $i < j$), acts on this Hilbert space in the usual way:

$$P_{ij}^{(m|n)} |s_1 \dots s_i \dots s_j \dots s_N\rangle = \epsilon_{ij}(\mathbf{s}) |s_1 \dots s_j \dots s_i \dots s_N\rangle\,, \tag{10.2}$$

The sign $\epsilon_{ij}(\mathbf{s}) \in \{\pm 1\}$ is 1 if both s_i and s_j are bosons, -1 if they are both fermions, and $(-1)^r$ if one of them is a boson and the other is a fermion, r being the number of fermions in the positions $i+1, \dots, j-1$. We shall also need in what follows the number operators $\mathcal{N}_\alpha$, defined by

$$\mathcal{N}_\alpha |\mathbf{s}\rangle = N_\alpha(\mathbf{s}) |\mathbf{s}\rangle, \tag{10.3}$$

where N_α is the number of particles with spin s_α in the basis state $|\mathbf{s}\rangle$.

We are now ready to write the Hamiltonian of the model:

$$\mathcal{H} = \sum_{i<j} J_{ij}(1 - P_{ij}^{(m|n)}) - \sum_{\alpha=1}^{m+n-1} \mu_\alpha \mathcal{N}_\alpha \equiv \mathcal{H}_0 + \mathcal{H}_1 \tag{10.4}$$

The first term $\mathcal{H}_0$ is a spin chain Hamiltonian, while the coefficient μ_α in the second term can be regarded as the chemical potential of the α-th species. We shall study the supersymmetric version of integrable Haldane–Shastry spin chains of A_{N-1} type, for which the coupling constants J_{ij} are given by

$$\frac{J}{2\sin^2(\xi_i^{\mathrm{HS}} - \xi_j^{\mathrm{HS}})}, \quad \frac{J}{(\xi_i^{\mathrm{PF}} - \xi_j^{\mathrm{PF}})^2}, \quad \frac{J}{2\sinh^2(\xi_i^{\mathrm{FI}} - \xi_j^{\mathrm{FI}})} \tag{10.5}$$

In the latter equation $J \neq 0$ is a real constant, $\xi_i^{\mathrm{HS}} = i\pi/N$, ξ_i^{PF} are the zeros of the Hermite polynomial of degree N and $\mathrm{e}^{2\xi_i^{\mathrm{FI}}}$ are the zeros of the Laguerre polynomial L_N^{c-1} with $c > 0$. A set of symmetries of this Hamiltonian (relating the su$(m|n)$ and su$(n|m)$ models with suitable values of the chemical potentials μ_α) can be readily found, but we will not insist in these details here. The interested reader can find a complete discussion in [19].

10.3 Partition Function and Spectrum

The partition function provides a compact way of expressing the spectrum of the model under study. Its computation will be carried as is customary with this type of models by exploiting their relation with the dynamical spin models of Calogero–Sutherland type (to be precise, of A_{N-1} type) through the Polychronakos freezing trick.

The spin models of Calogero–Sutherland type are constructed as a generalization of the well-known scalar models. In the simplest (rational) case, the scalar Calogero model [14] Hamiltonian is given by

$$H_{\mathrm{sc}} = -\sum_i \partial_{x_i}^2 + a^2 \sum_i x_i^2 + \sum_{i \neq j} \frac{a(a-1)}{(x_i - x_j)^2} \tag{10.6}$$

Introducing the spin interaction using spin exchange operators (in our case, of supersymmetric type) we obtain the Hamiltonian of the spin Calogero model:

$$H_0 = -\sum_i \partial_{x_i}^2 + a^2 \sum_i x_i^2 + \sum_{i \neq j} \frac{a(a - P_{ij}^{(m|n)})}{(x_i - x_j)^2} \tag{10.7}$$

Introducing the operator

$$h(\mathbf{x}) = J \sum_{i<j} \frac{1 - P_{ij}^{(m|n)}}{(x_i - x_j)^2} - \sum_{\alpha=1}^{m+n-1} \mu_\alpha \mathcal{N}_\alpha \tag{10.8}$$

which yields the Hamiltonian of the PF spin chain when the coordinates (dynamical variables) x_i are replaced by the chain sites ξ_i, we can write

$$H \equiv H_0 + \frac{2a}{J}\mathcal{H}_1 = H_{\mathrm{sc}} + \frac{2a}{J} h(\mathbf{x}) \tag{10.9}$$

When $a \to \infty$, the eigenfunctions of the Hamiltonian H concentrate around the coordinates of the equilibrium position of the scalar potential

$$U(\mathbf{x}) = \sum_i x_i^2 + \sum_{i \neq j} \frac{1}{(x_i - x_j)^2} \tag{10.10}$$

which can be easily proved to be unique (in the configuration space $A = \{\mathbf{x} \in \mathbf{R}^N : x_1 < \cdots < x_N\}$) and coincide with the zeros of the Hermite polynomial of degree N, that is, the chain sites. By (10.9), the energies of H are then approximately given by

$$E_{ij} \simeq E_i + \frac{2a}{j} e_j$$

where E_i and e_j respectively denote the energies of the scalar Calogero model and the spin chain (10.4). The latter equation cannot be directly used to solve for the energies e_j, since we don't know a priori how the energies of the spin Hamiltonian (10.9) combine with those of the scalar Calogero model. Instead, we can exploit this equation in order to express the partition function $\mathcal{Z}$ of the spin chain as the $a \to \infty$ limit of the quotient of the partition functions of the dynamical spin model and the scalar one, namely

$$\mathcal{Z}(T) = \lim_{a \to \infty} \frac{Z(2aT/J)}{Z_{\mathrm{sc}}(2aT/J)} \tag{10.11}$$

This is the essence of Polychronakos's freezing trick.

The computation of the partition function of the scalar model is straightforward, with the result

$$\lim_{a \to \infty} q^{-JE_{\mathrm{GS}}/(2a)} Z_{\mathrm{sc}}(2aT/J) = \prod_i (1 - q^{iJ})^{-1}, \quad q \equiv \mathrm{e}^{-1/T} \tag{10.12}$$

where

$$E_{\mathrm{GS}} = aN + a^2 N(N-1) \tag{10.13}$$

is the ground state energy of both the scalar and the spin Calogero model. On the other hand, the computation of the partition function of the spin dynamical model (with a chemical potential) is rather involved and here we will only outline it, referring to [19] for the complete details. We shall first compute the spectrum of H_0 and then, since H_0 and $\mathcal{H}_1$ obviously commute, we will easily obtain the spectrum of H.

To begin with, we extend symmetrically the configuration space from the Weyl chamber A to the whole space $\mathbf{R}^N$. The extension is equivalent to the original Hamiltonian (they have the same spectrum) provided that we symmetrize the wave functions of the extended Hamiltonian. More precisely, if Λ denotes the total symmetrizer with respect to both the spatial and spin coordinates (taking care of the supersymmetric character of the model), it can be proved that H is given by an upper triangular matrix in a basis with states of the form

$$|\mathbf{n}, \mathbf{s}\rangle = \Lambda\Big(\rho(\mathbf{x}) \prod_i x_i^{n_i} |\mathbf{s}\rangle\Big), \quad \rho(\mathbf{x}) = \mathrm{e}^{-\frac{a}{2}\sum_i x_i^2} \prod_{i<j} |x_i - x_j|^a \tag{10.14}$$

where $\mathbf{n} = (n_1, \ldots, n_N)$ with $n_i \in \mathbf{Z}_{\geq 0}$. Note that ρ is simply the ground state of the scalar Calogero model. In fact, in order to select a basis among these states we have to impose some restrictions due to their symmetry under permutations, namely

(i) $n_i \geq n_{i+1}$, $i = 1, \ldots, N-1$
(ii) if $n_i = n_{i+1}$ then $s_i \leq s_{i+1}$ if s_i is bosonic or $s_i < s_i + 1$ if s_i is fermionic

The energies of the Hamiltonian H_0, which can be directly read from the diagonal of this matrix, are given by

$$E^0_{\mathbf{n},\mathbf{s}} = 2a|\mathbf{n}| + E_{\mathrm{GS}}, \quad |\mathbf{n}| = \sum_i n_i \tag{10.15}$$

Since $\mathcal{H}_1$ is obviously diagonal in the above basis, namely

$$\mathcal{H}_1|\mathbf{n}, \mathbf{s}\rangle = -\Big(\sum_i \mu_{s_i}\Big)|\mathbf{n}, \mathbf{s}\rangle \tag{10.16}$$

the spectrum of the full Hamiltonian H is simply

$$E_{\mathbf{n},\mathbf{s}} = 2a|\mathbf{n}| - \frac{2a}{J}\sum_i \mu_{s_i} + E_{\mathrm{GS}} \tag{10.17}$$

In order to compute the partition function of H, we still have to determine the (intrinsic) degeneracies of the energy levels just found. Since $E_{\mathbf{n},\mathbf{s}}$ is independent of $\mathbf{s}$, these are simply the number of spin configurations $\mathbf{s}$ compatible with a given multiindex $\mathbf{n}$ according to the above two rules. The procedure in this kind of supersymmetric models is based on the close relation of these degeneracies with the two standard families (complete and elementary) of symmetric polynomials in N variables, respectively denoted by $h_i(\mathbf{x})$ and $e_i(\mathbf{x})$, and to their supersymmetric extensions defined by

$$E_k(x_1, \ldots, x_m|y_1, \ldots, y_n) = \sum_{i+j=k} h_i(x_1, \ldots, x_m)e_j(y_1, \ldots, y_n) \tag{10.18}$$

(see, e.g., [30]). The partition function can then be written as [19]

$$\lim_{a\to\infty} q^{-JE_{\mathrm{GS}}/(2a)}Z(2aT/J) = \sum_{\mathbf{k}\in\mathcal{P}_N} \Sigma(\mathbf{k})q^{\sum_{i=1}^{r-1} JK_i}\prod_{i=1}^{r}(1-q^{JK_i})^{-1} \tag{10.19}$$

where $\mathcal{P}_N$ are the ordered partitions of N (of any allowed length r), $\mathbf{k} = (k_1, \ldots, k_r)$ and $K_i = \sum_{j=1}^{i} k_j$. The term $\Sigma(\mathbf{k})$, which takes care of the degeneracy of the energy levels, is given by

$$\begin{aligned}\Sigma(\mathbf{k}) &\equiv E_{\mathbf{k}}(q^{-\mu_1},\dots,q^{-\mu_m}|q^{-\mu_{m+1}},\dots,q^{-\mu_{m+n}})\\ &= \prod_{i=1}^{r} e_{k_i}(q^{-\mu_1},\dots,q^{-\mu_m}|q^{-\mu_{m+1}},\dots,q^{-\mu_{m+n}})\end{aligned}$$

with $\mu_{m+n}=0$. This construction is based on the properties of the symmetric polynomials and their supersymmetric counterparts, and in particular on the fact that the value of h at the point $(1,\dots,1)$ is the number of combinations with repetitions while the value of e at the same point is the number of combinations [30]. We can now construct the partition function of the spin chain (10.4) with rational interactions (10.5) by taking the quotient of the partition functions (10.19) and (10.12), with the result

$$\mathcal{Z}(T)=\sum_{\mathbf{k}\in\mathcal{P}_N}\Sigma(\mathbf{k})q^{\sum_{i=1}^{r-1}JK_i}\prod_{i=1}^{N-r}\left(1-q^{JK_i'}\right) \tag{10.20}$$

where $\{K_1',\dots,K_{N-r}'\}=\{1,\dots,N-1\}\setminus\{K_1,\dots,K_{r-1}\}$. By repeating the same procedure with the trigonometric and hyperbolic interactions (10.5), we finally obtain the following remarkable formula for the partition function of all three chains of HS type (10.4)–(10.5):

$$\mathcal{Z}(T)=\sum_{\mathbf{k}\in\mathcal{P}_N}\Sigma(\mathbf{k})q^{\sum_{i=1}^{r-1}J\mathcal{E}(K_i)}\prod_{i=1}^{N-r}\left(1-q^{J\mathcal{E}(K_i')}\right) \tag{10.21}$$

where the *dispersion function* $\mathcal{E}$ is given by

$$\begin{aligned}\mathcal{E}_{\mathrm{HS}}(i)&=i(N-1)\\ \mathcal{E}_{\mathrm{PF}}(i)&=i\\ \mathcal{E}_{\mathrm{FI}}(i)&=i(i+c-1)\end{aligned}$$

The latter expression for the partition function contains all the information needed to study the spectrum. Given m and n, the number of degrees of freedom of bosons and fermions, and the number of particles N, we can find the energy levels and their degeneracies. In fact, this expression can be easily implemented in a symbolic manipulation program. However, this form of the partition function is not suitable for the study of the thermodynamics of the chain, as we would need to take its limit when N goes to infinity and this cannot be easily achieved. We shall instead show the equivalence of the Hamiltonian (10.4)–(10.5) with a suitable vertex model. This will allow us to write the partition function in a form suited for studying the thermodynamic properties of our model.

The vertex model referred to above is a one-dimensional array of $N+1$ sites and N links which can take one of m possible bosonic or n fermionic values. A state can thus be described by a *bond vector* $\boldsymbol{\sigma}=(\sigma_1,\dots,\sigma_N)$, where σ_i is the value of the bond i. The energy of such a configuration σ is then defined as

$$E^{(m|n)}(\sigma) = J \sum_{i=1}^{N-1} \delta(\sigma_i, \sigma_{i+1}) \mathcal{E}(i) \tag{10.22}$$

where $\mathcal{E}(i)$ is the dispersion relation previously found for each of our chain models and $\delta(i, j)$ is 0 when $i < j$ or $i = j$ is a bosonic value, and 1 if $i > j$ or $i = j$ is fermionic. Let us now define, following [10], the generalized partition function

$$\mathcal{Z}^V(q; \mathbf{x}|\mathbf{y}) = \sum_{\sigma_1,\ldots,\sigma_N=1}^{m+n} \prod_{\alpha=1}^{m} x_\alpha^{N_\alpha(\sigma)} \prod_{\beta=1}^{n} y_\beta^{N_{m+\beta}(\sigma)} \, q^{E^{(m|n)}(\sigma)} \tag{10.23}$$

where $N_\alpha(\sigma)$ is the number of bonds in the vector σ equal to α, in terms of which the partition function $\mathcal{Z}^V$ of the vertex model with energy (10.22) is given by

$$\mathcal{Z}^V(q) = \mathcal{Z}^V(q; 1, \ldots, 1|1, \ldots, 1) \tag{10.24}$$

The usefulness of the vertex model is brought out by showing that its generalized partition function gives, for a particular value of the variables $(\mathbf{x}, \mathbf{y})$, the partition function of our spin chains:

$$\mathcal{Z}(q) = \mathcal{Z}^V(q; q^{-\mu_1}, \ldots, q^{-\mu_m}|q^{-\mu_{m+1}}, \ldots, q^{-\mu_{m+n}}) \tag{10.25}$$

This result follows from an alternative form of expressing the generalized partition function in terms of Schur polynomials [30], namely

$$\mathcal{Z}^V(q; \mathbf{x}|\mathbf{y}) = \sum_{\mathbf{k}\in\mathcal{P}_N} S_{\mathbf{k}}(\mathbf{x}|\mathbf{y}) q^{\sum_{i=1}^{r-1} J\mathcal{E}(K_i)} \tag{10.26}$$

and the identity

$$\sum_{\mathbf{k}\in\mathcal{P}_N} S_{\mathbf{k}}(\mathbf{x}|\mathbf{y}) q^{\sum_{i=1}^{r-1} J\mathcal{E}(K_i)} = \sum_{\mathbf{k}\in\mathcal{P}_N} E_{\mathbf{k}}(\mathbf{x}|\mathbf{y}) \, q^{\sum_{i=1}^{r-1} J\mathcal{E}(K_i)} \prod_{i=1}^{N-r} \left(1 - q^{J\mathcal{E}(K_i')}\right) \tag{10.27}$$

proved in [8] and [10]. Comparing with (10.21) we easily obtain (10.25), which can equivalently be written as

$$\mathcal{Z}(q) = \sum_{\sigma_1,\ldots,\sigma_N=1}^{m+n} q^{E^{(m|n)}(\sigma) - \sum_{\alpha=1}^{m+n} \mu_\alpha N_\alpha(\sigma)} \tag{10.28}$$

As a consequence, the spectrum can be expressed in terms of the supersymmetric version of Haldane's motifs [8, 10, 26], $\delta_i(\sigma) \equiv \delta(\sigma_i, \sigma_{i+1})$, as

$$E(\sigma) = E^{(m|n)}(\sigma) - \sum_{\alpha=1}^{m+n} \mu_\alpha N_\alpha(\sigma) = J \sum_{i=1}^{N-1} \delta_i(\sigma)\, \mathcal{E}(i) - \sum_i \mu_{\sigma_i}. \tag{10.29}$$

This is the equation we shall use in the next section to study the thermodynamics of the supersymmetric chains (10.4)–(10.5).

10.4 The Free Energy

Since we are interested in the behavior of the thermodynamic functions when $N \to \infty$, we need to rescale the coupling constant of the model to ensure that the extensive functions become proportional to N in this limit. For instance, for the PF chain

$$\sum_{i=1}^{N-1} \mathcal{E}(i) = \frac{1}{2} N(N-1) \tag{10.30}$$

so that we should choose the coupling constant as $J = K/N$ with $K =$ constant in order that the mean energy remains finite when $N \to \infty$. Of course, similar results hold for the PF and FI chains (see [19]). We then define a rescaled dispersion relation

$$\varepsilon(x_i) = \frac{J}{K}\, \mathcal{E}(i), \qquad \text{with} \quad \varepsilon(x) = x, \quad x_i = \frac{i}{N} \tag{10.31}$$

To compute the free energy we will use a generalization of the transfer matrix method. To this end, we first write the energy (10.29) in terms of the rescaled dispersion relation, as

$$E(\sigma) = \sum_{i=1}^{N-1} \Big[K\delta(\sigma_i, \sigma_{i+1})\varepsilon(x_i) - \frac{1}{2}(\mu_{\sigma_i} + \mu_{\sigma_{i+1}}) \Big] - \frac{1}{2}(\mu_{\sigma_1} + \mu_{\sigma_N}) \tag{10.32}$$

and if $A(x)$ is the matrix defined by its elements:

$$A_{\alpha\beta}(x) = q^{K\varepsilon(x)\delta(\alpha,\beta) - \frac{1}{2}(\mu_\alpha + \mu_\beta)}, \quad \alpha, \beta = 1, \ldots, m+n \tag{10.33}$$

the partition function can be written as the trace of a product of these matrices:

$$\mathcal{Z}(q) = \mathrm{tr}\big[A(x_0)A(x_1)\ldots A(x_{N-1})\big] \tag{10.34}$$

The easiest case would correspond to $A(x_i) \equiv A_i$ being diagonal, since the product and the trace are then trivially computed. Although this is not the case for our models, we can at least convert A_i into its Jordan form J_i. It is not hard to prove that the matrices P_k turning A_k into their Jordan form satisfy $P_i^{-1} P_{i+1} = \mathbf{1} + \mathrm{O}(N^{-1})$. It can then be

shown that when $N \to \infty$ the free energy per site

$$f(T) = -(T/N) \log \mathcal{Z}$$

behaves as

$$f(T) \simeq -\frac{T}{N} \log \mathrm{tr}(UJ_0 \dots J_{N-1}), \quad U = \lim_{N\to\infty} P_{N-1}^{-1} P_0 \tag{10.35}$$

We will now assume that the matrix $J_0 \dots J_{N-1}$ is diagonal, as can be shown to be the case for the su(1|1) models we shall mainly deal with in this report. In that case

$$\mathrm{tr}(UJ_0 \dots J_{N-1}) = \sum_{\alpha=1}^{m+n} U_{\alpha\alpha} \Lambda_\alpha, \quad \Lambda_\alpha = \prod_{i=0}^{N-1} \lambda_\alpha(x_i) \tag{10.36}$$

where $\lambda_\alpha(x_i)$ are the eigenvalues of $A(x_i)$. A straightforward argument, based on the fact that the elements of $A(x)$ are strictly positive and the application of the Perron–Frobenius theorem, leads to the approximate equality

$$\mathrm{tr}(UJ_0 \dots J_{N-1}) \simeq U_{11} \prod_{i=0}^{N-1} \lambda_1(x_i) \tag{10.37}$$

where $\lambda_1(x_i)$ is the largest eigenvalue (in module) of $A(x_i)$ (simple and positive). The free energy per site can be written in the thermodynamic limit as:

$$f(T) = -T \lim_{N\to\infty} \frac{1}{N} \sum_{i=0}^{N-1} \log \lambda_1(x_i) = -T \int_0^1 \log \lambda_1(x) \mathrm{d}x \tag{10.38}$$

This simple expression [valid for all the models discussed in this report, as well as other models with energies given by an expression of the form (10.29)] allows for a complete study of the thermodynamic properties of these chains. All the standard thermodynamic functions such as the density of spins of a given type, the internal energy, the heat capacity and the entropy can be easily computed once the free energy is known. In the next section we will study in some detail the simplest case of supersymmetric spin chains of HS type, namely the su(1|1) models.

10.5 The su(1|1) Supersymmetric Spin Chain

We will consider in this section the simplest case $m = n = 1$ of the supersymmetric spin chains (10.4)–(10.5). Due to the symmetry properties of these chains [19], we can actually restrict our attention to the case $K > 0$. The 2×2 matrix A in this case is simply given by

$$A(x) = \begin{pmatrix} q^{-\mu} & q^{-\mu/2} \\ q^{K\varepsilon(x)-\mu/2} & q^{K\varepsilon(x)} \end{pmatrix} \tag{10.39}$$

where $\mu = \mu_1$ is the only chemical potential of this model. The matrix has a zero eigenvalue, the other one being

$$\lambda_1 = q^{K\varepsilon(x)} + q^{-\mu} \tag{10.40}$$

and is therefore diagonalizable. The free energy is then given by (10.38), which in this case reads

$$f(T,\mu) = -\mu - T\int_0^1 \log\left(1 + \mathrm{e}^{-\beta(K\varepsilon(x)+\mu)}\right)\mathrm{d}x \tag{10.41}$$

Note that, in contrast with previous approaches based on the equivalence of the spin chain (10.4) of HS type with a free fermion model (see, e.g., [15]), this formula is valid for all three families of HS chains under study.

We will next analyze the critical behavior of the su(1|1) chains of HS type. To this end, recall [1, 12] that as $T \to 0$ the free energy density of a $1+1$ dimensional CFT behaves as

$$f(T) \simeq f(0) - \frac{\pi c T^2}{6v} \tag{10.42}$$

with v the effective speed of light (Fermi velocity) and c the central charge of the theory. Ascertaining that this asymptotic behavior also holds for the free energy per site (10.41) of the su(1|1) chains will provide a strong indication of their criticality, i.e., their conformal invariance, and allow us to determine their central charge as a function of the chemical potential μ and the coupling constant K.

First of all, it is easy to check that if $\mu > 0$, there is no critical behavior (we are considering the case $K > 0$). In fact, in this case, $K\epsilon(x) + \mu$ is a positive quantity for all x in the interval $[0, 1]$ and we have

$$|f(T,\mu) - f(0,\mu)| < T\int_0^1 \mathrm{e}^{-\beta(K\varepsilon(x)+\mu)}\mathrm{d}x < T\mathrm{e}^{-\beta\mu} \tag{10.43}$$

which proves that the system is not critical. It is also straightforward to show that if $\mu < -K\varepsilon_{\max}$, where $\varepsilon_{\max}$ is the maximum of the rescaled dispersion relation in the interval $[0, 1]$, the behavior of the free energy (10.41) when $T \to 0$ does not match that of a CFT. Thus we only need to study three cases, $\mu \in (-K\varepsilon_{\max}, 0)$, $\mu = -K\varepsilon_{\max}$ and $\mu = 0$.

Let us first consider the case $-K\varepsilon_{\max} < \mu < 0$. To get a result valid for the three chains, using the symmetry properties of the dispersion relation, we will write the free energy as:

$$f(T,\mu) + \mu = -\eta T\int_0^{1/\eta} \log\left(1 + \mathrm{e}^{-\beta(K\varepsilon(x)+\mu)}\right)\mathrm{d}x \tag{10.44}$$

where $\eta = 2$ for the HS chain and 1 for PF and FI chains. By studying the sign of the exponent of the integrand in this equation we can recast it in the form

$$f(T,\mu) - f(\mu,0) = -\eta T \int_0^{1/\eta} \log\left(1 + \mathrm{e}^{-\beta|K\varepsilon(x)+\mu|}\right)\mathrm{d}x \tag{10.45}$$

Clearly, the main contribution to the integral comes from a neighborhood of the unique root x_0 of the equation $K\varepsilon(x) + \mu = 0$ in the interval $(0, 1/\eta)$. Indeed, it is obvious that the rescaled dispersion relation is monotonically increasing in the interval $(0, 1/\eta)$ for all three chains of HS type, and the condition $-K\varepsilon_{\max} < \mu < 0$ implies that $-\mu/K$ is in the range of $\varepsilon(x)$ in this interval. If $\Delta < \min(x_0, 1/\eta - x_0)$, the expression

$$I(T) = \int_{x_0-\Delta}^{x_0+\Delta} \log\left(1 + \mathrm{e}^{-\beta|K\varepsilon(x)+\mu|}\right)\mathrm{d}x \tag{10.46}$$

approximates the integral in (10.45) with an error given by

$$\int_A \log\left(1 + \mathrm{e}^{-\beta|K\varepsilon(x)+\mu|}\right)\mathrm{d}x < \int_A \mathrm{e}^{-\beta|K\varepsilon(x)+\mu|}\mathrm{d}x < \mathrm{e}^{-\beta\kappa} \tag{10.47}$$

where $A = [0, 1/\delta] \setminus (x_0 - \Delta, x_0 + \Delta)$ and $\kappa = \min(-\mu - \varepsilon(x_0 - \Delta), \mu + \varepsilon(x_0 + \Delta))$. The change of variables:

$$y = \beta|K\varepsilon(x) + \mu| \tag{10.48}$$

in each of the intervals $[x_0 - \Delta, x_0]$ and $[x_0, x_0 + \Delta]$ and a Taylor expansion of the factor $1/\varepsilon'(x)$ in a neighborhood of x_0:

$$\frac{1}{\varepsilon'(x)} = \frac{1}{\varepsilon'(x_0)} + \mathrm{O}(Ty) \tag{10.49}$$

allows us to write the integral (10.46) as

$$I(T) = \frac{2T}{K\varepsilon'(x_0)} \int_0^{\infty} \log(1 + \mathrm{e}^{-y})\mathrm{d}y + \mathrm{O}(T^2) = \frac{\pi^2 T}{6K\varepsilon'(x_0)} + \mathrm{O}(T^2) \tag{10.50}$$

(indeed, the error incurred in extending the integration interval to $+\infty$ is $\mathrm{O}(\mathrm{e}^{-\kappa'\beta})$). Thus the asymptotic behavior of the free energy per site (10.41) at low temperatures is

$$f(T,\mu) = f(0,\mu) - \frac{\eta\pi^2 T^2}{6K\varepsilon'(x_0)} + \mathrm{O}(T^3) \tag{10.51}$$

The effective speed of light is proportional in the three types of chains (10.5) to the derivative of the dispersion relation with respect to the momentum at the point x_0. Some subtle differences appear between the HS chain and the PF and FI chains, since

in these last cases the chains are not translationally invariant. We shall only quote here the final result, namely

$$v = \frac{K\epsilon'(x_0)}{\eta\pi} \tag{10.52}$$

(see [19] for the details). The final expression for the behavior of the free energy per site at low temperatures is thus

$$f(T,\mu) = f(0,\mu) - \frac{\pi T^2}{6v} + \mathrm{O}(T^3) \tag{10.53}$$

This strongly suggests that when $-K\varepsilon_{\max} < \mu < 0$ the three su(1|1) chains of HS type are critical, with central charge $c = 1$ corresponding to a free CFT with one bosonic field.

The endpoints $\mu = -K\varepsilon_{\max}$ and $\mu = 0$ can be examined in a similar fashion. At $\mu = 0$, the three chains are critical (provided that $\gamma \neq 0$ for the FI chain) with central charge $c = \frac{1}{2}$, a free CFT with a fermionic field. If $\gamma = \mu = 0$ the FI chain is not critical. At the other endpoint, $\mu = -K\varepsilon_{\max}$, the PF and FI chains are again critical with $c = \frac{1}{2}$, while the HS chain is not (in agreement with [15]).

10.6 Conclusions

We have discussed in this report some recent results on the critical behavior of supersymmetric spin chains of HS type. A more complete study appears in [19], where the su(2|1) and su(2|2) cases have also been dealt with in detail. Since the analytic expression (10.38) for the free energy is based on the knowledge of the largest eigenvalue of the $(m+n) \times (m+n)$ matrix A, it is clear that the complexity of the calculations greatly increases with these two parameters. However, as shown in [19], an explicit formula for the free energy can also be derived in the su(2|1) and su(2|2) cases. In particular, in the su(2|1) case a complete phase diagram (in the two-dimensional space parametrized by the chemical potentials of the two bosonic states) has been derived, showing the existence of critical regions with central charges which are not integers or half-integers. It has also been found in this case that the phase transitions are of first order type (discontinuous) in the bosonic densities for $K > 0$ (see, again, [19] for the details).

Future work in this field will be dedicated to the study of the existence of first-order transitions at $T = 0$ when $m + n > 2$, with particular emphasis on the $mn = 0$ case, that is, purely bosonic or fermionic chains with su(k) spin degrees of freedom. It turns to be that the study of these spin chains presents more difficulties that their supersymmetric counterparts. In fact, to the best of our knowledge only the su(2) case has been completely studied [16]. Note, finally, that the supersymmetric chains considered in this report are of A_{N-1} type, in the classification of these models

based on their relation to the spin Calogero–Sutherland models. The extension of the above results to spin chains associated to other root systems, as for instance BC_N case, certainly deserves further attention.

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Chapter 11
Towards a Quantum Sampling Theory: The Case of Finite Groups

Antonio G. García, Miguel A. Hernández-Medina and Alberto Ibort

Abstract Nyquist-Shannon sampling theorem, instrumental in classical telecommunication technologies, is extended to quantum systems supporting a unitary representation of a finite group G. Two main ideas from the classical theory having natural counterparts in the quantum setting: frames and invariant subspaces, provide the mathematical background for the theory. The main ingredients of classical sampling theorems are discussed and their quantum counterparts are thoroughly analyzed in this simple situation. A few examples illustrating the obtained results are discussed.

11.1 Introduction

Shannon's celebrated theorems: Shannon-Hartley's channel capacity theorem [18, 29], Shannon's source coding theorem [28] and Nyquist-Shannon sampling theorem [25, 29], constitute the backbone of the mathematical background of modern telecommunication technologies. The development of Quantum Information Technologies have caused that the first two theorems have already been extended to the quantum setting (see for instance [9, 32] and references therein) and their quantum counterparts are today part of the mainstream of Quantum Information.

A. G. García (✉)
Department of Mathematics, Universidad Carlos III de Madrid, Av. Universidad 30, 28911 Leganés-Madrid, Spain
e-mail: agarcia@math.uc3m.es

M. A. Hernández-Medina
Departamento de Matemática Aplicada a las Tecnologías de la Información y las Comunicaciones, E.T.S.I.T., U.P.M., Avda. Complutense 30, 28040 Madrid, Spain
e-mail: miguelangel.hernandez.medina@upm.es

A. Ibort
ICMAT and Department of Mathematics, Universidad Carlos III de Madrid, Av. Universidad 30, 28911 Leganés-Madrid, Spain
e-mail: albertoi@math.uc3m.es

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_11

Interestingly enough, Nyquist-Shannon sampling theorem has not found a place in Quantum Information yet. Actually, as far as we know, there is not a genuine quantum version of it. The classical sampling theorem states, in its more streamlined form, that band-limited signals $f(t)$ (within the interval $[-\pi, \pi]$ for instance) can be reconstructed from the family of samples $\{f(k)\}$ and a given family of signals $S_k(t)$, k being an integer. More precisely:

$$f(t) = \sum_{k\in\mathbb{Z}} f(k) \frac{\sin \pi(t-k)}{\pi(t-k)}, \qquad t \in \mathbb{R}. \tag{11.1}$$

It is obvious the interest that sampling formulas, similar to the previous one, would have in the quantum setting as they would provide an alternative way to describe the states of quantum systems. Thus, if we consider, instead of signals, vectors $|x\rangle$ in a Hilbert space describing pure states of a quantum system, a "quantum sampling theorem" would provide a way of reconstructing the states from a family of "samples", denoted in what follows by $\{\mathcal{L}x(k)\}$, k an index, and a prescribed set of quantum states $\{|C_k\rangle\}$, the analogues of the signals $\left\{S_k(t) = \frac{\sin \pi(t-k)}{\pi(t-k)}\right\}$ in classical sampling theory, (11.1), as $|x\rangle = \sum_k \mathcal{L}x(k)|C_k\rangle$. Such auxiliary states could be manufactured independently of the system under scrutiny and all that would be needed will be to prepare a superposition of them with coefficients the previously obtained samples.

Arguably, it can be stated that any orthonormal basis $\{|e_k\rangle\}$ provides a sampling theorem with samples the amplitudes $\mathcal{L}x(k) = \langle e_k|x\rangle$ and with auxiliary states the orthonormal vectors themselves, i.e., $|C_k\rangle = |e_k\rangle$. Actually, Shannon's formula (11.1) is just the orthonormal expansion in the Hilbert space of square integrable functions in the real line of the function f with respect to the orthonormal basis $\{S_k\}$. Notice however that the orthonormal basis given by the shifted sine-cardinal functions $S_k(t) = \frac{\sin \pi(t-k)}{\pi(t-k)}$ has the additional property that the coefficients of the expansion are the actual values of the function f itself, and the word "sample" has, in this context, the meaning of the actual value of the function which is precisely the fact that provides the ground for its technological implementation and it is one of the main properties of Shannon's theorem that we would like to extend to the quantum setting.

We must point out that, certainly, quantum tomography (see for instance [4, 19] and references therein) aims also in the direction sketched above, however the current status of the theory doesn't allow for a clear cut reconstruction theorem as the ones provides by Shannon's theorem and its generalizations.

Thus the aim of the present paper is to walk the first steps into the construction of a rigorous and broad enough sampling theory for quantum systems inspired directly in the classical sampling theorem by Nyquist-Shannon. In order to achieve it, we will use some recent ideas underlying a family of classical generalized Shannon's theorems. Two ingredients appearing in these generalizations seem to be critical for the development of a quantum version: the use of frames and shift-invariant subspaces [16].

Frames provide a convenient and flexible tool extending the notion of orthonormal or Riesz bases in Hilbert spaces [8]. Traditionally, frames were used in signal and image processing, non-harmonic analysis, data compression, and sampling theory, but nowadays frame theory plays also a fundamental role in a wide variety of problems in both pure and applied mathematics, computer science, physics and engineering. Let us recall that a frame is any sequence of vectors $\{|c_k\rangle\}$ in a Hilbert space such that there exist two constants $0 < A \leq B$ such that for any vector $|x\rangle$ we have

$$A||x||^2 \leq \sum_k |\langle c_k \mid x\rangle|^2 \leq B||x||^2 .$$

Given a frame $\{|c_k\rangle\}$ in a Hilbert space the representation property of any vector $|x\rangle$ as a series $|x\rangle = \sum_k \alpha_k |c_k\rangle$ is retained, but, unlike the case of orthonormal (Riesz) bases, the uniqueness of this representation (for overcomplete frames) is sacrificed. Suitable frame coefficients α_k which depend continuously and linearly on $|x\rangle$ are obtained by using dual frames $\{|d_k\rangle\}$ of $\{|c_k\rangle\}$, i.e., $\{|d_k\rangle\}$ is another frame for the Hilbert space such that $|x\rangle = \sum_k \langle d_k \mid x\rangle\, |c_k\rangle = \sum_k \langle c_k \mid x\rangle\, |d_k\rangle$. Recall that a Riesz basis in a separable Hilbert space is the image of an orthonormal basis by means of a bounded invertible operator; a Riesz basis has a unique dual (biorthogonal) basis. A Riesz sequence in a Hilbert space is a Riesz basis for its closed span. For more details on the theory of frames see, for instance, the monograph [8] and references therein.

The redundancy of frames, which gives flexibility and robustness, is the key to their significance for applications (see, for instance, the nice introduction in Chap. 1 of [7] and references therein). It is worth to note that frames in finite dimension are nothing but spanning sets of vectors. Frames have already been considered in problems related to this work (see for instance [2, 3], or more recently [5]).

The second ingredient consists of a natural extension of the notion of shift-invariant subspaces of $L^2(\mathbb{R})$, that is, subspaces of functions invariant under the shift transformation $f(t) \mapsto f(t-1)$, that play a fundamental role in classical sampling theory [16] (see also [1, 30]). The shift transformation defines a unitary operator on the Hilbert space of square integrable functions on the real line. Hence it is natural to consider subspaces of a Hilbert space which are invariant under a given unitary transformation U and to extend to this situation the results of classical sampling theory. This idea has been recently considered in a number of papers (see for instance the related works [11–13, 15, 24, 27]).

More concretely, to visualize better the role of these two ingredients and to prepare the ground for the sampling theorem to be derived in this paper, let us describe the generalized classical sampling theorem that can be obtained combining them and that we want to extend to the quantum setting. Indeed, let V_{samp} be the Hilbert space where we want to obtain a sampling formula involving the sequence $\{m_k(x)\}$ of measurements (samples) obtained from each $|x\rangle \in V_{\text{samp}}$. The general mathematical procedure can be summarized as follows (see [12, 14, 16] for details):

1. Determine and auxiliary L^2-Hilbert space, denoted simply by L^2, and an isomorphism $\mathcal{T}_V : L^2 \to V_{\text{samp}}$.
2. Express the available samples $\{m_k(x)\}$ of $|x\rangle \in V_{\text{samp}}$ as the inner products $m_k(x) = \langle f_k \mid f\rangle_{L^2}$ where $\{f_k\}$ is some fixed sequence in L^2, and $|x\rangle$ is the image under $\mathcal{T}_V$ of the function f.
3. Characterize the above sequence $\{f_k\}$ as a frame for the L^2-auxiliary space.
4. Find the dual frames $\{g_k\}$ of $\{f_k\}$. Thus we have

$$f = \sum_k \langle f_k \mid f\rangle\, g_k = \sum_k m_k(x)\, g_k\,.$$

5. Finally, applying the isomorphism $\mathcal{T}_V$ in the above expansion we get a sampling formula in V_{samp}. Namely,

$$|x\rangle = \sum_k m_k(x)\, |\mathcal{T}_V(g_k)\rangle\,.$$

Moreover, due to the unitary invariant character of V_{samp}, the isomorphism $\mathcal{T}_V$ satisfies a *shifting property* which simplifies the obtention of the reconstruction vectors $|\mathcal{T}_V(g_k)\rangle$.

In the particular case of the classical sampling theorem, (11.1), we have that any band-limited function f can be expressed as

$$f(t) = \Big\langle \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-i\pi wt} \big| \widehat{f} \Big\rangle_{L^2[-\pi,\pi]}\,, \quad t \in \mathbb{R}\,, \tag{11.2}$$

where $\widehat{f}$ denotes the Fourier transform of f. In particular, for the samples of f at $k \in \mathbb{Z}$ we have that $f(k) = \big\langle \mathrm{e}^{-i\pi kt}/\sqrt{2\pi} \mid \widehat{f}\,\big\rangle_{L^2[-\pi,\pi]}$, and the isomorphism $\mathcal{T}_V$ is the inverse Fourier transform $\mathcal{F}^{-1}$. Since the sequence $\big\{\mathrm{e}^{-i\pi kt}/\sqrt{2\pi}\big\}_{k\in\mathbb{Z}}$ is an orthonormal basis for $L^2[-\pi,\pi]$ we have

$$\widehat{f}(w) = \sum_{k\in\mathbb{Z}} f(k)\, \frac{\mathrm{e}^{-i\pi kw}}{\sqrt{2\pi}} \qquad \text{in } L^2[-\pi,\pi]\,,$$

and applying $\mathcal{F}^{-1}$,

$$f(t) = \sum_{k\in\mathbb{Z}} f(k)\, \mathcal{F}^{-1}\Big(\frac{\mathrm{e}^{-i\pi kw}}{\sqrt{2\pi}}\, \chi_{[-\pi,\pi]}(w)\Big)(t) = \sum_{k\in\mathbb{Z}} f(k)\, \frac{\sin\pi(t-k)}{\pi(t-k)} \quad \text{in } L^2(\mathbb{R})\,.$$

Notice that we have used that $\mathcal{F}^{-1}\big(\chi_{[-\pi,\pi]}(w)\big)(t) = \frac{\sin\pi t}{\pi t}$ and the shifting property which satisfies the Fourier transform. Cauchy-Schwarz's inequality in (11.2) proves the inequality $|f(t)| \le \|f\|$, $t \in \mathbb{R}$. In other words, here the convergence in norm implies pointwise convergence which is uniform on $\mathbb{R}$.

Classical sampling has been generalized in the following way: In $L^2(\mathbb{R})$ consider the shift operator $U : f(t) \mapsto f(t-1)$. The functions (signals) to be sampled belong to some (principal) shift-invariant subspace $V_\varphi^2 := \overline{\text{span}}_{L^2(\mathbb{R})}\{\varphi(t-n),\ n \in \mathbb{Z}\}$, where the generator function φ belongs to $L^2(\mathbb{R})$ and the sequence $\{\varphi(t-n)\}_{n\in\mathbb{Z}}$ is a Riesz sequence for $L^2(\mathbb{R})$. Thus, the shift-invariant space V_φ^2 can be described as

$$V_\varphi^2 = \Big\{ \sum_{n\in\mathbb{Z}} \alpha_n\, \varphi(t-n) \ :\ \{\alpha_n\}_{n\in\mathbb{Z}} \in \ell^2(\mathbb{Z}) \Big\}$$

In particular, spline or wavelet spaces are examples of shift-invariant subspaces V_φ^2.

On the other hand, in many common situations the available data are samples of some filtered versions $f * \mathsf{h}_j$ of the signal f itself, where the average function h_j reflects the characteristics of the acquisition device. For N convolution systems (linear time-invariant systems or filters in engineering jargon) $\mathcal{L}_j f := f * \mathsf{h}_j$, $j = 1, 2, \ldots, N$, assume that, for any f in V_φ^2, the sequence of samples $\{(\mathcal{L}_j f)(rm)\}_{m\in\mathbb{Z};\, j=1,2,\ldots,N}$ is available, where $r \in \mathbb{N}$ denotes the sampling period. The generalized sampling problem mathematically consists of the stable recovery of any $f \in V_\varphi^2$ from the above sequence of its samples. In other words, it deals with the construction of sampling formulas in V_φ^2 having the form

$$f(t) = \sum_{j=1}^{N} \sum_{m\in\mathbb{Z}} \big(\mathcal{L}_j f\big)(rm)\, S_j(t - rm)\,, \qquad t \in \mathbb{R}\,, \tag{11.3}$$

where the sequence of reconstruction functions $\{S_j(\cdot - rm)\}_{m\in\mathbb{Z};\, j=1,2,\ldots,N}$ is a frame for the shift-invariant space V_φ^2. In this setting, the isomorphism $\mathcal{T}_{V_\varphi^2} : L^2(0,1) \to V_\varphi^2$ maps the orthonormal basis $\{\mathrm{e}^{-2\pi inw}\}_{n\in\mathbb{Z}}$ onto $\{\varphi(t-n)\}_{n\in\mathbb{Z}}$, and it satisfies the shifting property $\mathcal{T}_{V_\varphi^2}(e^{-2\pi inx}F) = (\mathcal{T}_{V_\varphi^2}F)(t-n)$ for $F \in L^2(0,1)$, $n \in \mathbb{Z}$. Similar results can be obtained if we consider a unitary operator U in an abstract Hilbert space instead of the shift operator in $L^2(\mathbb{R})$ (see [11, 12, 27]).

In this paper we will consider an extension of the previous generalized sampling formula, (11.3), to the realm of an abstract complex separable Hilbert space $\mathcal{H}$ whose rays represent the pure states of a quantum system. The notion of U-invariant subspaces will be extracted from a situation which is common in physical systems and that corresponds to the presence of a group represented unitarily on the state space of the system. That is, we will consider a group G and a unitary representation $U : G \to \mathcal{U}(\mathcal{H})$. Hence, the main notion that will be used henceforth will be that of subspaces invariant under the representation of the group G, i.e., closed subspaces $W \subset \mathcal{H}$ such that $U(g)W \subset W$ for all $g \in G$. Clearly the notion of U-invariant subspace corresponds to the choice of the Abelian group of integers $\mathbb{Z}$ and the unitary representation provided by $U(n) = U^n$ where U is a given unitary operator. The theory developed in what follows can also be considered as a non-commutative extension of the standard classical sampling theory once we restrict ourselves to Hilbert spaces which are Hilbert spaces of functions defined on a suitable measure space.

Only finite groups G will be discussed here, both for simplicity of exposition and because many relevant physical systems exhibit them in a natural way as symmetry groups: from chemistry and molecular physics [6, 21, 31], to condensed matter physics [10]. It is worth to point it out that it is not necessary that the group G would be a symmetry group of the system. Actually, if the group is a symmetry group, we will get and additional information on the form of a sampling formula for the time-evolution of the given state, however, in order to construct the sampling expansions exhibited below, is unnecessary.

The use of frames, finite under the circumstances, will be natural within this context. The auxiliary space used in the theory will be the space of square integrable functions in the group, that in this context agrees with the group algebra of the group G.

The first part of the paper, Sect. 11.2, will be devoted to establish the mathematical setting of the problem, to discuss the main ideas used later on, like the notion frames. and to introduce the main notion of generalized samples and their properties. In Sect. 11.3 the main theorem stating the sampling formula for a family of states of quantum systems supporting an unitary representation of a finite group will be established. Finally, in Sect. 11.4 some illustrative examples will be discussed, in particular the simple cases of cyclic and dihedral groups which are fundamental in the applications of the theory.

11.2 The Mathematical Setting

Let G be a finite (not necessarily commutative) group with identity element e; we denote its order as $|G|$. Let also $g \in G \mapsto U(g) \in \mathcal{U}(\mathcal{H})$ be a unitary representation of a G in a complex separable Hilbert space $\mathcal{H}$, i.e., a homomorphism from the groups G into the group $\mathcal{U}(\mathcal{H})$ of unitary operators on $\mathcal{H}$. Notice that because the group G is finite any unitary representation is completely reducible into finite dimensional irreducible components. However, for reasons that will be clear along the text, it will be better to decompose the Hilbert space $\mathcal{H}$ in cyclic invariant subspaces, that is, invariant subspaces W possessing a cyclic vector $|a\rangle$, hence $W = \text{span}\{U(g)|a\rangle \mid g \in G\}$: Notice that because G is finite the cyclic vector spaces $\mathcal{H}_a$ are finite-dimensional. We will denote such space by $\mathcal{H}_a$ and it is clear that $\mathcal{H}$ can be decomposed as a countable direct sum of mutually orthogonal such subspaces $\mathcal{H} = \bigoplus_{n=1}^{\infty} \mathcal{H}_n$, $\mathcal{H}_n = \mathcal{H}_{a_n}$, for a family of vectors $a_n \in \mathcal{H}$. Consequently the problem of sampling a given state $|x\rangle \in \mathcal{H}$ is reduced to the problem of sampling the components $|x_n\rangle \in \mathcal{H}_{a_n}$ such that $|x\rangle = \sum_n |x_n\rangle$.

So, from now on, we will consider a fixed vector $|a\rangle \in \mathcal{H}$ and the subspace $\mathcal{H}_a$ of $\mathcal{H}$ spanned by $U(g)|a\rangle$, $g \in G$. Sometimes, for convenience, the vector $U(g)|a\rangle$ will be denoted either as $|ga\rangle$ or $|a_g\rangle$. In case the set $\{|ga\rangle \mid g \in G\}$ is linearly independent in $\mathcal{H}$, each $|x\rangle \in \mathcal{H}_a$ can be expressed as the unique expansion $|x\rangle = \sum_{g\in G} \alpha_g U(g)|a\rangle$, with $\alpha_g \in \mathbb{C}$, in which case we will say that the representation U is faithful. Notice that if we denote by U_a the restriction of the action of G to the subspace $\mathcal{H}_a$, the subset $G_0 = \{g \in G \mid U_a(g)|x\rangle = |x\rangle, \forall |x\rangle \in \mathcal{H}_a\}$ is a normal

subgroup of G and the quotient group G/G_0 acts faithfully in $\mathcal{H}_a$, i.e., there is a natural unitary representation $\tilde{U}$ defined on G/G_0 as $\tilde{U}(gG_0)|a\rangle = U(g)|a\rangle$, such that the family of vectors $\tilde{U}(gG_0)|a\rangle$ is linearly independent. Thus, in what follows, we will assume that the unitary representation of the group G on the subspace $\mathcal{H}$ is faithful.

There is a close relationship between the (finite) sequence $|a_g\rangle = U(g)|a\rangle$ and the so-called *stationary sequences* (see Kolmogorov [23]). We say that the sequence $\{|x_g\rangle \,:\, g \in G\}$ in $\mathcal{H}$ is (left) G-*stationary* if:

$$\langle x_g|x_{g'}\rangle_{\mathcal{H}} = \langle x_{hg}|x_{hg'}\rangle_{\mathcal{H}}\,, \qquad \forall g, g', h \in G\,.$$

Then it is easy to deduce, provided that the vectors $|x_g\rangle$ are linearly independent, that there exists a unitary representation $U(g)$ of G and an $|a\rangle = |x_e\rangle \in \mathcal{H}$ such that $|x_g\rangle = U(g)|a\rangle$, $g \in G$. Thus we define the *auto-covariance* of the finite sequence $\big\{U(g)|a\rangle = |ga\rangle\big\}_{g\in G}$ as $R_a(g) := \langle a|ga\rangle_{\mathcal{H}}$, $g \in G$. Similarly, we can define the *cross-covariance* between the finite sequences $\big\{U(g)|a\rangle\big\}_{g\in G}$ and $\big\{U(g)|b\rangle\big\}_{g\in G}$ where $|a\rangle, |b\rangle \in \mathcal{H}$ as

$$R_{a,b}(g) := \langle a|gb\rangle_{\mathcal{H}}\,, \quad g \in G\,.$$

Note that $R_{a,b}(g) = \overline{R_{b,a}(g^{-1})}$ for $|a\rangle, |b\rangle \in \mathcal{H}$ and $g \in G$.

Proposition 1 *Let $R_a\colon G \to \mathbb{C}$ denote the function defined by the auto-covariance of the sequence $U(g)|a\rangle$, $g \in G$. Then the function R_a is of nonnegative type. Moreover the function R_a will be positive definite iff the representation U is faithful or, equivalently, if $\mathbf{R}_a$ denotes the $|G| \times |G|$ square matrix $\big(R_a(h^{-1}g)\big)_{(h,g)\in G\times G}$, the set of vectors $\big\{U(g)|a\rangle \,:\, g \in G\big\}$ is linearly independent in $\mathcal{H}$ if and only if* $\det \mathbf{R}_a \neq 0$.

Proof A function $\varphi\colon G \to \mathbb{C}$ is said to be of nonnegative type if for any finite family g_i, $i = 1, \ldots, N$ of group elements and complex numbers ζ_i, it is verified that $\sum_{i,j=1}^{N} \bar{\zeta}_i \zeta_j \varphi(g_i^{-1} g_j) \geq 0$. Hence we get that

$$\sum_{i,j=1}^{N} \bar{\zeta}_i \zeta_j R_a(g_i^{-1} g_j) = \left(\sum_{i=1}^{N} \bar{\zeta}_i \langle g_i a|\right)\left(\sum_{j=1}^{N} \zeta_j |g_j a\rangle\right) \geq 0\,.$$

Then notice that the function R_a will be positive iff $\sum_{j=1}^{N} \zeta_j |g_j a\rangle \neq 0$ for all ζ_i.

Equivalently, if $\det \mathbf{R}_a = 0$ then there exists a vector $\boldsymbol{\lambda} = (\lambda_g)_{g\in G} \in \mathbb{C}^{|G|}$ such that $\boldsymbol{\lambda} \neq \mathbf{0}$ and $\mathbf{R}_a\boldsymbol{\lambda} = 0$. Thus $\sum_{g\in G} \lambda_g |ga\rangle$ is orthogonal to $|ga\rangle$ for all $g \in G$ so that $\sum_g \lambda_g\, |ga\rangle = 0$. Conversely, if $\sum_{g\in G} \lambda_g\, |ga\rangle = 0$ for some $\boldsymbol{\lambda} \neq \mathbf{0}$ then the inner product in the above expression with each $|ha\rangle$, $h \in G$, yields $\mathbf{R}_a\boldsymbol{\lambda} = 0$. □

The natural isomorphism $\mathcal{T}_a^G$

Consider the group algebra $\mathbb{C}[G]$, that is, the (finite dimensional) complex linear space generated by the elements of the group G. Thus $\mathbb{C}[G]$ has dimension $|G|$ and

its elements can be identified with the space of functions $\boldsymbol{\alpha}\colon G \to \mathbb{C}$, $g \mapsto \boldsymbol{\alpha}(g)$; in brief $\boldsymbol{\alpha} = \big(\boldsymbol{\alpha}(g)\big)_{g\in G}$. In the case we are dealing here of finite groups, such functions are all obviously integrable and square integrable, hence it can be identified with $L^2(G)$ that endowed with its natural inner product $\langle \boldsymbol{\alpha} \mid \boldsymbol{\beta}\rangle$ becomes a Hilbert space isomorphic to $\mathbb{C}^{|G|}$.

The Hilbert space $L^2(G)$ supports a natural unitary representations of G called the *left regular representation* L_s, $s \in G$, defined by (similarly on the right):

$$L_s\boldsymbol{\alpha}(g) = \boldsymbol{\alpha}(s^{-1}g) \quad \text{for } s, g \in G\,.$$

Next we define the following isomorphism $\mathcal{T}_a^G$ (corresponding to the isomorphism $\mathcal{T}_V$ used in classical sampling theory discussed in (i) in the introduction) between $L^2(G)$ and $\mathcal{H}_a$:

$$\begin{aligned} \mathcal{T}_a^G\colon L^2(G) &\longrightarrow \mathcal{H}_a \\ \boldsymbol{\alpha} &\longmapsto |x\rangle = \sum_{g\in G} \boldsymbol{\alpha}(g)\, U(g)|a\rangle\,. \end{aligned} \tag{11.4}$$

Notice that $\mathcal{T}_a^G$ is an isomorphism because of the assumption that the representation of G on $\mathcal{H}_a$ is faithful. In what follows, if there is no risk of confussion, we will simply denote it by $\mathcal{T}$.

This isomorphism $\mathcal{T}$ has the following *shifting property* with respect to the left regular representation L_s:

Proposition 2 *For any $s \in G$ and $\boldsymbol{\alpha} \in L^2(G)$ we have that*

$$\mathcal{T}\big(L_s\boldsymbol{\alpha}\big) = U(s)\,\mathcal{T}(\boldsymbol{\alpha}) \tag{11.5}$$

Proof Indeed, denoting $g' = s^{-1}g$ we have

$$\mathcal{T}\big(L_s\boldsymbol{\alpha}\big) = \sum_{g\in G} \boldsymbol{\alpha}(s^{-1}g)U(g)|a\rangle = \sum_{g'\in G} \boldsymbol{\alpha}(g')U(sg')|a\rangle \tag{11.6}$$

$$= \sum_{g'\in G} \boldsymbol{\alpha}(g')U(s)U(g')|a\rangle = U(s)\,\mathcal{T}(\boldsymbol{\alpha}) \tag{11.7}$$

□

Notice that the shifting property (11.5) is just the alluded shifting property in the introduction which is satisfied by the isomorphism $\mathcal{T}_V$.

An expression for the generalized samples

For our sampling purposes we consider an Abelian subgroup K of G (not necessarily normal) such that it possesses a *complement* H, i.e., H is a subgroup of G such that $KH = G$ and $K \cap H = \{e\}$ (in particular, K is a *transversal* of H). Notice that in such case both coset spaces G/H and $K\backslash G$ are bijective to K and H respectively (though not isomorphic as groups). Any group element $g \in G$ can be factorized uniquely as

$g = kh$ with $k \in K$ and $h \in H$. Then, to any coset gH we may associate the element $k \in H$ such that $g = kh$. This application is well defined because if $g'H = gH$, then $g' = gh'$, for some $h' \in H$, hence the factorization of g' becomes $g' = k(hh')$.

In case that K is a normal subgroup, the Schur-Zassenhaus theorem gives us a sufficient condition for the existence of a complement of K in G. Namely, if K is an Abelian normal subgroup of G such that $|K|$ and $|G/K|$ are coprime then there exists a complement H of K in G. For more details see, for instance, [20, p. 76]. In such case the group G is the *semidirect product* of K and H, and denoted as $G = K \rtimes H$. Moreover if G is the semidirect product of the Abelian subgroup K (not necessarily normal) and the normal subgroup H, i.e., $G = H \rtimes K$, then $G = HK$, $K \cap H = \{e\}$ and H is a complement of K. Notice that in such case the natural identification $K \cong G/H$ is an actual group isomorphism. This is a situation which is commonly found in applications to specific physical systems with the group G a kynematical group.

Because of the canonical identification discussed above between G/H and K, we can choose an element of K associated to any coset of the quotient set G/H. Thus, denoting $\ell := |K| = |G|/|H|$, in case $K = \{k_0 = e, k_1, \ldots, k_{\ell-1}\}$, we can describe the quotient set G/H as:

$$G/H = \{H, k_1 H, \ldots, k_{\ell-1} H\} .$$

From now on we write the group G as (for any fixed way of writing the elements of H)

$$G = \bigcup_{j=0}^{\ell-1} k_j^{-1} H .$$

Fixed N elements $b_j \in \mathcal{H}$, $j = 1, 2, \ldots, N$, for each $|x\rangle = \sum_{s\in G} \alpha_s U(s)|a\rangle \in \mathcal{H}_a$ we define its *generalized samples* by

$$\mathcal{L}_j x(k_n) := \langle U(k_n) b_j \mid x \rangle_{\mathcal{H}} , \quad n = 0, 1, \ldots, \ell - 1 \quad \text{and} \quad j = 1, 2, \ldots, N . \tag{11.8}$$

We will refer to each $\mathcal{L}_j$ as a $\mathcal{L}_j$-system acting on $\mathcal{H}_a$, $j = 1, 2, \ldots, N$.

Notice that the expression for the generalized samples (11.8) is an straightforward generalization of the convolution of the sampled vector $|x\rangle$ with the vectors $|b_j\rangle$.

Besides, to recover any $|x\rangle \in \mathcal{H}_a$ we need at least $|G|$ samples; if we are sampling at K, we will need at least N $\mathcal{L}_j$-systems such that $N\ell \geq |G| = \ell|H|$, i.e., $N \geq |H|$.

As it was discussed in the introduction, the main goal of this paper is to recover any state vector $|x\rangle \in \mathcal{H}_a$ by means of its generalized samples (11.8) and sampling formulas taking care of the unitary structure of $\mathcal{H}_a$. To this end, we first obtain an alternative expression for the generalized sample $\mathcal{L}_j x(k_n)$ with $n = 0, 1, \ldots, \ell - 1$. Namely,

$$\begin{aligned}\mathcal{L}_j x(k_n) &= \langle U(k_n)b_j \mid x\rangle_{\mathcal{H}} = \Big\langle U(k_n)b_j \mid \textstyle\sum_{s\in G}\alpha_s\, U(s)a\Big\rangle_{\mathcal{H}} \\ &= \textstyle\sum_{s\in G}\alpha_s \langle U(k_n)b_j \mid U(s)a\rangle_{\mathcal{H}} = \langle G_{j,k_n} \mid \boldsymbol{\alpha}\rangle_{L^2(G)}\,, \end{aligned} \tag{11.9}$$

where $\boldsymbol{\alpha} = (\alpha_s)_{s\in G}$ and $G_{j,k_n} = (\overline{\langle U(k_n)b_j \mid U(g)a\rangle})_{g\in G} = \langle (k_n^{-1}g)a \mid b_j\rangle_{g\in G}$ belong to $L^2(G)$.

The vectors $G_{j,k_n} \in L^2(G)$, $j = 1, 2, \ldots, N$, $n = 0, 1, \ldots, \ell - 1$, can be expressed, in terms of the cross-covariances $R_{b_j,a}$, as

$$G_{j,k_n} = \big(\overline{R_{b_j,a}(k_n^{-1}s)}\big)_{s\in G}\,. \tag{11.10}$$

Having in mind expression (11.9) for the samples and the isomorphism $\mathcal{T}_a^G$ defined in (11.4) we deduce the following result (see also the finite frame theory in [7]):

Proposition 3 *Any $|x\rangle \in \mathcal{H}_a$ can be recovered from its samples $\{\mathcal{L}_j x(k_n)\}$, $j = 1, 2, \ldots, N$, $n = 0, 1, \ldots, \ell - 1$ if and only if the set of vectors $\{G_{j,k_n}\}$, $j = 1, 2, \ldots, N$, $n = 0, 1, \ldots, \ell - 1$, in $L^2(G)$ form a frame (a spanning set) for $L^2(G)$.*

Equivalently, the $|G| \times N\ell$ matrix

$$\begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ G_{1,k_0} & \cdots & G_{1,k_{\ell-1}} & G_{2,k_0} & \cdots & G_{2,k_{\ell-1}} & \cdots & G_{N,k_0} & \cdots & G_{N,k_{\ell-1}} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} \tag{11.11}$$

has rank $|G|$. Hence, we have that $|G| \le N\ell$, that is, the number of needed $\mathcal{L}_j$-systems is necessarily $N \ge |H|$. The vectors G_{j,k_n} can be written as column matrices as

$$G_{j,k_n} = \Big(\overline{R_{b_j,a}}(k_n^{-1}k_0^{-1}H), \overline{Rb_j, a}(k_n^{-1}k_1^{-1}H), \ldots, \overline{Rb_j, a}(k_n^{-1}k_{\ell-1}^{-1}H)\Big)^{\top}$$

where $k_n \in K$ and $\overline{R_{b_j,a}}(k_n^{-1}k_p^{-1}H)$ is given by

$$\overline{R_{b_j,a}}(k_n^{-1}k_p^{-1}H) = \Big(\overline{R_{b_j,a}}(k_n^{-1}g_{p_1}), \overline{R_{b_j,a}}(k_n^{-1}g_{p_2}), \ldots, \overline{R_{b_j,a}}(k_n^{-1}g_{p_{|H|}})\Big)$$

being $k_p^{-1}H = \{g_{p_1}, \ldots, g_{p_{|H|}}\}$ with $p = 0, 1, \ldots, \ell - 1$.

For each $j = 1, 2, \ldots, N$ let $\mathbf{R}_{b_j,a}$ be the $\ell \times |G|$ matrix

$$\mathbf{R}_{b_j,a} = \begin{pmatrix} R_{b_j,a}(k_0^{-1}k_0^{-1}H) & R_{b_j,a}(k_0^{-1}k_1^{-1}H) & \ldots & R_{b_j,a}(k_0^{-1}k_{\ell-1}^{-1}H) \\ R_{b_j,a}(k_1^{-1}k_0^{-1}H) & R_{b_j,a}(k_1^{-1}k_1^{-1}H) & \ldots & R_{b_j,a}(k_1^{-1}k_{\ell-1}^{-1}H) \\ \vdots & \vdots & \cdots & \vdots \\ R_{b_j,a}(k_{\ell-1}^{-1}k_0^{-1}H) & R_{b_j,a}(k_{\ell-1}^{-1}k_1^{-1}H) & \ldots & R_{b_j,a}(k_{\ell-1}^{-1}k_{\ell-1}^{-1}H) \end{pmatrix}$$

Since K is an Abelian subgroup of G the cosets $k_n^{-1}k_p^{-1}H$ and $k_p^{-1}k_n^{-1}H$ coincide. As a consequence, $\mathbf{R}_{b_j,a}$ is the block symmetric matrix

$$\mathbf{R}_{b_j,a} = \begin{pmatrix} R_{b_j,a}(k_0^{-1}k_0^{-1}H) & R_{b_j,a}(k_1^{-1}k_0^{-1}H) & \dots & R_{b_j,a}(k_{\ell-1}^{-1}k_0^{-1}H) \\ R_{b_j,a}(k_0^{-1}k_1^{-1}H) & R_{b_j,a}(k_1^{-1}k_1^{-1}H) & \dots & R_{b_j,a}(k_{\ell-1}^{-1}k_1^{-1}H) \\ \vdots & \vdots & \dots & \vdots \\ R_{b_j,a}(k_0^{-1}k_{\ell-1}^{-1}H) & R_{b_j,a}(k_1^{-1}k_{\ell-1}^{-1}H) & \dots & R_{b_j,a}(k_{\ell-1}^{-1}k_{\ell-1}^{-1}H) \end{pmatrix} \tag{11.12}$$

The matrix given in (11.11) can be written as $\left(\mathbf{R}_{b_1,a}^* \mathbf{R}_{b_2,a}^* \dots \mathbf{R}_{b_N,a}^*\right)$, where the symbol $*$ denotes the transpose conjugate matrix. Thus, Proposition 3 can be restated in terms of the $N\ell \times |G|$ matrix of cross-covariances $\mathbf{R}_{\mathbf{b},a}$ defined by

$$\mathbf{R}_{\mathbf{b},a} := \begin{pmatrix} \mathbf{R}_{b_1,a} \\ \mathbf{R}_{b_2,a} \\ \vdots \\ \mathbf{R}_{b_N,a} \end{pmatrix}. \tag{11.13}$$

Corollary 1 *Any* $|x\rangle \in \mathcal{H}_a$ *can be recovered from its samples* $\left\{\mathcal{L}_j x(k_n)\right\}$, $j = 1, 2, \dots, N$, $n = 0, 1, \dots, \ell - 1$ *if and only* rank $\mathbf{R}_{\mathbf{b},a} = |G|$.

Besides, (11.9) can be expressed, for any $|x\rangle = \sum_{s\in G} \alpha_s U(s)|a\rangle$ in $\mathcal{H}_a$, as

$$\begin{pmatrix} \mathcal{L}_j x(k_0) \\ \mathcal{L}_j x(k_1) \\ \vdots \\ \mathcal{L}_j x(k_{\ell-1}) \end{pmatrix} = \mathbf{R}_{b_j,a}\, \boldsymbol{\alpha}$$

where $\boldsymbol{\alpha} = (\alpha_s)_{s\in G}$. As a consequence we deduce the samples expression:

Proposition 4 *For any* $|x\rangle = \sum_{s\in G} \alpha_s U(s)|a\rangle$ *in* $\mathcal{H}_a$ *consider its samples vector*

$$\mathcal{L}_{\text{samp}} x = \left(\mathcal{L}_1 x(k_0) \dots \mathcal{L}_1 x(k_{\ell-1}) \dots \mathcal{L}_N x(k_0) \dots \mathcal{L}_N x(k_{\ell-1})\right)^\top. \tag{11.14}$$

Then, the matrix relationship

$$\mathcal{L}_{\text{samp}} x = \mathbf{R}_{a,\mathbf{b}}\, \boldsymbol{\alpha} \tag{11.15}$$

holds, where $\boldsymbol{\alpha} = (\alpha_s)_{s\in G}$ *and* $\mathbf{R}_{\mathbf{b},a}$ *is the* $N\ell \times |G|$ *matrix of cross-covariances defined in (11.13).*

Assuming that $\{G_{j,k_n}\}, j = 1, 2, \dots, N, n = 0, 1, \dots, \ell - 1$, is a frame for $L^2(G)$ we have that the rank of the matrix $\mathbf{R}_{\mathbf{b},a}$ is $|G|$. Thus the Moore-Penrose pseudoinverse of $\mathbf{R}_{\mathbf{b},a}$ is the $|G| \times N\ell$ matrix $\mathbf{R}_{\mathbf{b},a}^+ = [\mathbf{R}_{\mathbf{b},a}^* \mathbf{R}_{\mathbf{b},a}]^{-1} \mathbf{R}_{\mathbf{b},a}^*$ (see [26]). Writing the columns of $\mathbf{R}_{\mathbf{b},a}^+$ as

$$\mathbf{R}^{+}_{\mathbf{b},a} = \begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{R}^{+}_{1,k_0} & \cdots & \mathbf{R}^{+}_{1,k_{\ell-1}} & \mathbf{R}^{+}_{2,k_0} & \cdots & \mathbf{R}^{+}_{2,k_{\ell-1}} & \cdots & \mathbf{R}^{+}_{N,k_0} & \cdots & \mathbf{R}^{+}_{N,k_{\ell-1}} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

from (11.15) we obtain

$$\boldsymbol{\alpha} = \mathbf{R}^{+}_{\mathbf{b},a}\, \mathcal{L}_{\text{samp}} x = \sum_{j=1}^{N} \sum_{n=0}^{\ell-1} \mathcal{L}_j x(k_n) \mathbf{R}^{+}_{j,k_n} = \sum_{j=1}^{N} \sum_{n=0}^{\ell-1} \langle G_{j,k_n} \mid \boldsymbol{\alpha} \rangle_{L^2(G)} \mathbf{R}^{+}_{j,k_n} \tag{11.16}$$

In particular we derive that $\operatorname{rank} \mathbf{R}^{+}_{\mathbf{b},a} = |G|$ and that the columns of $\mathbf{R}^{+}_{\mathbf{b},a}$ form a dual frame of $\{G_{j,k_n}\}, j = 1, 2, \ldots, N, n = 0, 1, \ldots, \ell - 1$. Any other dual frame of $\{G_{j,k_n}\}, j = 1, 2, \ldots, N, n = 0, 1, \ldots, \ell - 1$, in $L^2(G)$ is given by the columns of any left-inverse matrix $\mathbf{M}$ of the matrix $\mathbf{R}_{\mathbf{b},a}$. All these matrices are expressed as (see [26])

$$\mathbf{M} = \mathbf{R}^{+}_{\mathbf{b},a} + \mathbf{U}[\mathbf{I}_{N\ell} - \mathbf{R}_{\mathbf{b},a} \mathbf{R}^{+}_{\mathbf{b},a}] \tag{11.17}$$

where $\mathbf{U}$ denotes any arbitrary $|G| \times N\ell$ matrix.

11.3 The Sampling Result

Let $|x\rangle = \sum_{s \in G} \alpha_s\, U(s)|a\rangle$ a vector of $\mathcal{H}_a$; applying the isomorphism (11.4) in (11.16) we have

$$|x\rangle = \mathcal{T}(\boldsymbol{\alpha}) = \sum_{j=1}^{N} \sum_{n=0}^{\ell-1} \mathcal{L}_j x(k_n)\, \mathcal{T}(\mathbf{R}^{+}_{j,k_n})\,.$$

Similarly we may obtain a sampling formula like above for each left-inverse of $\mathbf{R}_{\mathbf{b},a}$ in (11.17). Indeed, denoting $\{\mathbf{m}_{j,k_n}\}, j = 1, 2, \ldots, N, n = 0, 1, \ldots, \ell - 1$, the columns of a left-inverse $\mathbf{M}$ of $\mathbf{R}_{\mathbf{b},a}$, one gets

$$|x\rangle = \sum_{j=1}^{N} \sum_{n=0}^{\ell-1} \mathcal{L}_j x(k_n)\, \mathcal{T}(\mathbf{m}_{j,k_n})\,. \tag{11.18}$$

The sampling functions $\mathcal{T}(\mathbf{m}_{j,k_n})$ in (11.18) do not have, in principle, any special structure for using the shifting property (11.5) since, in general, $\mathbf{M}$ does not have it. In the next section we construct specific left-inverses of $\mathbf{R}_{\mathbf{b},a}$ such that their associated sampling formulas take care of the unitary structure of $\mathcal{H}_a$.

G-compatible left-inverses

We denote by $\mathbf{S}$ the first $|H|$ rows of any left-inverse of the matrix $\mathbf{R}_{\mathbf{b},a}$ taken from (11.17); i.e,

$$\mathbf{S}\,\mathbf{R}_{\mathbf{b},a} = \left(\mathbf{I}_{|H|}\ \mathbf{O}_{|H|\times(|G|-|H|)}\right). \tag{11.19}$$

Having in mind the structure of $\mathbf{R}_{\mathbf{b},a}$ we write the $|H| \times N\ell$ matrix $\mathbf{S}$ as

$$\mathbf{S} = \left(\mathbf{S}_1\,\mathbf{S}_2 \ldots \mathbf{S}_N\right)$$

where each block $\mathbf{S}_j$ is a $|H| \times \ell$ matrix denoted by $\mathbf{S}_j = \left(S_j^0\, S_j^1\, \ldots\, S_j^{\ell-1}\right)$ where $S_j^n \in \mathbb{C}^{|H|}$ for each $n = 0, 1, \ldots, \ell-1$ and $j = 1, 2, \ldots, N$. From (11.12) and (11.19) we have:

$$\sum_{j=1}^{N}\sum_{n=0}^{\ell-1} S_j^n\, R_{b_j,a}(k_0^{-1}k_n^{-1}H) = \mathbf{I}_{|H|}$$

$$\sum_{j=1}^{N}\sum_{n=0}^{\ell-1} S_j^n\, R_{b_j,a}(k_k^{-1}k_n^{-1}H) = \mathbf{O}_{|H|}, \quad k = 1, 2, \ldots, \ell-1\,,$$

or equivalently

$$\sum_{j=1}^{N}\sum_{n=0}^{\ell-1} S_j^n\, R_{b_j,a}(k_n^{-1}H) = \mathbf{I}_{|H|} \tag{11.20}$$

$$\sum_{j=1}^{N}\sum_{n=0}^{\ell-1} S_j^n\, R_{b_j,a}(k_n^{-1}k_k^{-1}H) = \mathbf{O}_{|H|}, \quad k = 1, 2, \ldots, \ell-1\,. \tag{11.21}$$

Now, we form the $|G| \times N\ell$ matrix $\widetilde{\mathbf{S}} = \left(\widetilde{\mathbf{S}}_1\,\widetilde{\mathbf{S}}_2, \ldots \widetilde{\mathbf{S}}_N\right)$. Each $|G| \times \ell$ block $\widetilde{\mathbf{S}}_j$, $j = 1, 2, \ldots, N$, is formed from the columns of $\mathbf{S}_j$ in the following manner:

$$\widetilde{\mathbf{S}}_j := \begin{pmatrix} S_j^0 & S_j^1 & \cdots & S_j^{\ell-1} \\ S_j^{0,1} & S_j^{1,1} & \cdots & S_j^{\ell-1,1} \\ \vdots & \vdots & \cdots & \vdots \\ S_j^{0,\ell-1} & S_j^{1,\ell-1} & \cdots & S_j^{\ell-1,\ell-1} \end{pmatrix}$$

where, for $i = 1, 2, \ldots, \ell-1$ and $n, k = 0, 1, \ldots, \ell-1$, we set

$$S_j^{n,i} := S_j^k \quad \text{whenever } k_n^{-1}k_i^{-1} = k_k^{-1} (\text{or, equivalently, } k_i\,k_n = k_k)\,. \tag{11.22}$$

Lemma 1 *The above* $|G| \times N\ell$ *matrix* $\widetilde{\mathbf{S}}$ *is a left-inverse of* $\mathbf{R}_{\mathbf{b},a}$*, i.e,* $\widetilde{\mathbf{S}}\,\mathbf{R}_{\mathbf{b},a} = \mathbf{I}_{|G|}$.

Proof From (11.20) and (11.21), for each $i = 1, 2, \ldots, \ell - 1$, we have

$$\sum_{j=1}^{N}\sum_{n=0}^{\ell-1} S_j^{n,i}\, R_{b_j,a}(k_n^{-1}k_i^{-1}H) = \sum_{j=1}^{N}\sum_{k=0}^{\ell-1} S_j^{k}\, R_{b_j,a}(k_k^{-1}H) = \mathbf{I}_{|H|}$$

and

$$\sum_{j=1}^{N}\sum_{n=0}^{\ell-1} S_j^{n,i}\, R_{b_j,a}(k_n^{-1}k_p^{-1}H) = \sum_{j=1}^{N}\sum_{k=0}^{\ell-1} S_j^{k}\, R_{b_j,a}(k_n^{-1}k_p^{-1}H) = \mathbf{O}_{|H|}, \quad p \neq i\,.$$

As a consequence, we deduce that $\widetilde{\mathbf{S}}\,\mathbf{R}_{\mathbf{b},a} = \mathbf{I}_{|G|}$. □

It is worth to mention that, in particular, the Moore-Penrose pseudo-inverse $\mathbf{R}^{+}_{\mathbf{b},a}$ is a G-compatible left-inverse of $\mathbf{R}_{\mathbf{b},a}$; see [17] for the details.

Next we denote the columns of $\widetilde{\mathbf{S}}$ as

$$\widetilde{\mathbf{S}} = \begin{pmatrix} \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ \widetilde{\mathbf{S}}_{1,0} & \cdots & \widetilde{\mathbf{S}}_{1,\ell-1} & \widetilde{\mathbf{S}}_{2,0} & \cdots & \widetilde{\mathbf{S}}_{2,\ell-1} & \cdots & \widetilde{\mathbf{S}}_{N,0} & \cdots & \widetilde{\mathbf{S}}_{N,\ell-1} \\ \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots \end{pmatrix} \tag{11.23}$$

Using the left-inverse $\widetilde{\mathbf{S}}$ of $\mathbf{R}_{\mathbf{b},a}$ instead of $\mathbf{R}^{+}_{\mathbf{b},a}$ in (11.16), for each $|x\rangle = \sum_{s\in G} \alpha_s\, U(s)|a\rangle$ in $\mathcal{H}_a$ we obtain

$$\boldsymbol{\alpha} = \widetilde{\mathbf{S}}\,\mathcal{L}_{\text{samp}} = \sum_{j=1}^{N}\sum_{n=0}^{\ell-1} \mathcal{L}_j x(k_n)\,\widetilde{\mathbf{S}}_{j,n}\,.$$

Therefore,

$$|x\rangle = \mathcal{T}(\boldsymbol{\alpha}) = \sum_{j=1}^{N}\sum_{n=0}^{\ell-1} \mathcal{L}_j x(k_n)\,\mathcal{T}(\widetilde{\mathbf{S}}_{j,n})\,.$$

On the other hand, the columns $\widetilde{\mathbf{S}}_{j,n}$, $j = 1, 2, \ldots, N$ and $n = 0, 1, \ldots, \ell - 1$, as vectors of $L^2(G)$ satisfy, by construction, see (11.22), the crucial property (for our sampling purposes)

$$\widetilde{\mathbf{S}}_{j,n} = L_{k_n}\widetilde{\mathbf{S}}_{j,0}, \quad j = 1, 2, \ldots, N, \;\; n = 0, 1, \ldots, \ell - 1\,.$$

Hence, the shifting property (11.5) gives

$$|x\rangle = \sum_{j=1}^{N}\sum_{n=0}^{\ell-1} \mathcal{L}_j x(k_n)\, \mathcal{T}(\widetilde{\mathbf{S}}_{j,n}) = \sum_{j=1}^{N}\sum_{n=0}^{\ell-1} \mathcal{L}_j x(k_n)\, \mathcal{T}(L_{k_n}\widetilde{\mathbf{S}}_{j,0})$$
$$= \sum_{j=1}^{N}\sum_{n=0}^{\ell-1} \mathcal{L}_j x(k_n)\, U(k_n)\mathcal{T}(\widetilde{\mathbf{S}}_{j,0})\,.$$

Therefore, we have proved that, for any $|x\rangle \in \mathcal{H}_a$ the sampling expansion

$$|x\rangle = \sum_{j=1}^{N}\sum_{n=0}^{\ell-1} \mathcal{L}_j x(k_n)\, U(k_n)|c_j\rangle \tag{11.24}$$

holds, where $|c_j\rangle = \mathcal{T}(\widetilde{\mathbf{S}}_{j,0}) \in \mathcal{H}_a$, $j = 1, 2, \ldots, N$. Notice that we have obtained a sampling result of the desired form, (11.3), where the desired sampling vectors are given by $|C_n, j\rangle = U(k_n)|c_j\rangle$ and the generalized samples are obtained by convolution on $L^2(G)$ with the matrix of cross-covariances. In fact, collecting all the pieces we have obtained until now we have the following result:

Theorem 1 *Given the $N\ell \times |G|$ matrix $\mathbf{R}_{\mathbf{b},a}$ defined in (11.13), the following statements are equivalent:*

1. $\operatorname{rank} \mathbf{R}_{\mathbf{b},a} = |G|$
2. *There exists a $|H| \times N\ell$ matrix $\mathbf{S}$ such that*

$$\mathbf{S}\,\mathbf{R}_{\mathbf{b},a} = \left(\mathbf{I}_{|H|}\,\mathbf{O}_{|H|\times(|G|-|H|)}\right)$$

3. *There exist N vectors $|c_j\rangle \in \mathcal{H}_a$, $j = 1, 2, \ldots, N$, such that $\{U(k_n)|c_j\rangle\}$, $j = 1, 2, \ldots, N$, $n = 0, 1, \ldots, \ell - 1$ is a frame for $\mathcal{H}_a$, and for any $|x\rangle \in \mathcal{H}_a$ the expansion*

$$|x\rangle = \sum_{j=1}^{N}\sum_{n=0}^{\ell-1} \mathcal{L}_j x(k_n)\, U(k_n)|c_j\rangle$$

holds.

4. *There exists a frame $\{|C_{j,n}\rangle\}$, $j = 1, 2, \ldots, N$, $n = 0, 1, \ldots, \ell - 1$, in $\mathcal{H}_a$ such that, for each $|x\rangle \in \mathcal{H}_a$ the expansion*

$$|x\rangle = \sum_{j=1}^{N}\sum_{n=0}^{\ell-1} \mathcal{L}_j x(k_n)\, |C_{j,n}\rangle$$

holds.

Proof That condition (1) implies condition (2) and condition (2) implies condition (3) have been proved above. Obviously, condition (3) implies condition (4): take $|C_{j,n}\rangle = U(k_n)|c_j\rangle$ for $j = 1, 2, \ldots, N$ and $n = 0, 1, \ldots, \ell - 1$. Finally, as a consequence of Corollary 1, condition (4) implies condition (1). □

For the particular case where $N = |H|$ we obtain:

Corollary 2 *Assume that $N = |H|$ and consider the $|G| \times |G|$ matrix of cross-covariances $\mathbf{R}_{\mathbf{b},a}$ defined in (11.13). The following statements are equivalent:*

1. *The matrix $\mathbf{R}_{\mathbf{b},a}$ is invertible.*
2. *There exist $|H|$ unique elements $|c_j\rangle \in \mathcal{H}_a$, $j = 1, 2, \ldots, |H|$, such that the sequence $\{U(k_n)|c_j\rangle\}$, $j = 1, 2, \ldots, |H|$, $n = 0, 1, \ldots, \ell - 1$ is a basis for $\mathcal{H}_a$, and the expansion of any $|x\rangle \in \mathcal{H}_a$ with respect to this basis is*

$$|x\rangle = \sum_{j=1}^{|H|} \sum_{n=0}^{\ell-1} \mathcal{L}_j x(k_n)\, U(k_n)|c_j\rangle\,.$$

In this case the interpolation property $\mathcal{L}_j c_{j'}(k_n) = \delta_{j,j'}\,\delta_{n,0}$ holds, whenever $n = 0, 1, \ldots, \ell - 1$ and $j, j' = 1, 2, \ldots, |H|$.

Proof Notice that the inverse matrix $\mathbf{R}_{\mathbf{b},a}^{-1}$ has necessarily the structure of the matrix $\widetilde{\mathbf{S}}$ in (11.23). The uniqueness of the expansion with respect to a basis gives the interpolation property. □

Sampling the dynamics

So far, the group G has played no dynamical role, that is, if the dynamical evolution of the state $|x\rangle$ is given by the one-parameter group of unitary operator $U_t = \exp(-it\mathsf{H})$ defined by the Hamiltonian operator H, no assumption on the commutation relations of the operators $U(g)$ and H is made. However, if we assume that G is a symmetry group of the system, that is $[U(g), \mathsf{H}] = \mathsf{0}$ for all $g \in G$, then the evolution $x(t)$ of the initial state takes a particularly simple form. Actually $|x(t)\rangle = U_t|x\rangle$, then using (11.24), we get:

$$|x(t)\rangle = U_t|x\rangle = \sum_{j=1}^{N} \sum_{n=0}^{\ell-1} \mathcal{L}_j x(k_n)\, U(k_n) U_t|c_j\rangle = \sum_{j=1}^{N} \sum_{n=0}^{\ell-1} \mathcal{L}_j x(k_n)\, U(k_n)|c_j(t)\rangle\,,$$

where $|c_j(t)\rangle$ denotes the dynamical evolution of the states $|c_j\rangle, j = 1, 2, \ldots, N$. Thus the evolved state $|x(t)\rangle$ can be recovered from the initial samples and the evolved states $|c_j(t)\rangle, j = 1, 2, \ldots, N$.

11.4 Some Simple Examples

We will end up the discussion by illustrating the obtained results with two simple examples: the cyclic group $\mathbb{Z}_N$ and the dihedral group D_3, or the C_{3v} group in the molecular symmetry notation, which is the symmetry group of molecules such as ammonia or phosphorus oxycloride.

The cyclic group case

This case corresponds to that of a unitary operator $U : \mathcal{H} \to \mathcal{H}$ in a Hilbert space $\mathcal{H}$ such that for some $|a\rangle \in \mathcal{H}$ there exists $M \in \mathbb{N}$ satisfying $U^M|a\rangle = |a\rangle$ and the set $\{|a\rangle, U|a\rangle, U^2|a\rangle, \ldots, U^{M-1}|a\rangle\}$ is linearly independent in $\mathcal{H}$.

If we consider a positive integer r such that r divides M and denote $\ell = M/r$, the goal is to obtain finite frames in the subspace $\mathcal{H}_a = \left\{ \sum_{k=0}^{M-1} \alpha_k U^k a \,:\, \alpha_k \in \mathbb{C} \right\}$ of $\mathcal{H}$, having the form $\{U^{rn}|c_j\rangle\}, j = 1, 2, \ldots, N, n = 0, 1, \ldots, \ell - 1$ where $|c_j\rangle \in \mathcal{H}_a$, $j = 1, 2, \ldots, N$, such that any $|x\rangle \in \mathcal{H}_a$ can be recovered from the samples $\{\mathcal{L}_j x(rn) := \langle U^{rn} b_j \mid x\rangle_{\mathcal{H}}\}, j = 1, 2, \ldots, N$, $n = 0, 1, \ldots, \ell - 1$, by means of the sampling expansion

$$|x\rangle = \sum_{j=1}^{N} \sum_{n=0}^{\ell-1} \mathcal{L}_j x(rn)\, U^{rn}|c_j\rangle\,,$$

which takes care of the U-structure of $\mathcal{H}_a$. In this example we are considering the cyclic group $G := \mathbb{Z}_M$, the unitary representation $n \mapsto U(n) := U^n$ and its cyclid subgroup $H := \mathbb{Z}_r$. This particular case has been deeply studied in [13, 15].

A practical example taken from *Signal Processing* consists of the periodic extension of finite signals. Indeed, consider the space $\ell^2_M(\mathbb{Z})$ of M-periodic signals with inner product $\langle \mathbf{x} \mid \mathbf{y}\rangle_{\ell^2_M} = \sum_{m=0}^{M-1} \overline{x(m)}\, y(m)$. If we take, for instance, the M periodic signal $\mathbf{a} := (1, 0, \ldots, 0)$ and the cyclid shift operator

$$U : \mathbf{x} = \{x(m)\} \longmapsto U\mathbf{x} := \{x(m-1)\}$$

in $\ell^2_M(\mathbb{Z})$, we trivially obtain that $U^M \mathbf{a} = \mathbf{a}$ and $\mathcal{H}_{\mathbf{a}} = \ell^2_M(\mathbb{Z})$.

Fixed N signals $\mathbf{b}_j \in \ell^2_M, j = 1, 2, \ldots, N$, each sample of $\mathbf{x} \in \ell^2_M$ is obtained from the M-periodic convolution

$$\mathcal{L}_j \mathbf{x}(rn) := \langle U^{rn}\mathbf{b}_j \mid \mathbf{x}\rangle_{\ell^2_N} = \sum_{m=0}^{M-1} x(m)\, \overline{\mathbf{b}_j(m - rn)} = \big(\mathbf{x} * \mathbf{h}_j\big)(rn)\,, \quad n = 0, 1, \ldots, \ell\,,$$

where $\mathbf{h}_j(m) = \overline{\mathbf{b}_j(-m)}$, $m = 0, 1, \ldots, M-1$.

As the cross-covariance $R_{b_j,a}(m) = \langle \mathbf{b}_j \mid U^m \mathbf{a}\rangle_{\ell^2_N} = \overline{b_j(m)}$, each $\ell \times M$ block $\mathbf{R}_{b_j,a}, j = 1, 2, \ldots, N$, of the $N\ell \times M$ matrix $\mathbf{R}_{\mathbf{b},a}$ in (11.13) takes the form

$$\mathbf{R}_{b_j,a} = \begin{pmatrix} \overline{b_j(0)} & \overline{b_j(1)} & \cdots & \overline{b_j(M-1)} \\ \overline{b_j(M-r)} & \overline{b_j(M-r+1)} & \cdots & \overline{b_j(2M-r-1)} \\ \vdots & \vdots & \ddots & \vdots \\ \overline{b_j(M-r(\ell-1))} & \overline{b_j(M-r(\ell-1)+1)} & \cdots & \overline{b_j(2M-1-r(\ell-1))} \end{pmatrix}$$

where the sampling period r divides M and $\ell = M/r$. In case the rank of $\mathbf{R}_{\mathbf{b},a}$ is M, which implies $N \geq r$ convolution systems, from Theorem 1 we obtain in $\ell^2_M(\mathbb{Z})$ a sampling formula as

$$\mathbf{x}(m) = \sum_{j=1}^{N} \sum_{n=0}^{\ell-1} \mathcal{L}_j \mathbf{x}(rn)\, \mathbf{c}_j(m-rn) = \sum_{j=1}^{N} \sum_{n=0}^{\ell-1} \big(\mathbf{x} * \mathbf{h}_j\big)(rn)\, \mathbf{c}_j(m-rn)\,,$$

where $m = 0, 1, \ldots, M-1$. The sampling sequences in $\ell^2_M(\mathbb{Z})$ are $\mathbf{c}_j = \mathcal{T}_a^G\big(\widetilde{\mathbf{S}}_{j,0}\big)$, $j = 1, 2, \ldots, s$, where $\widetilde{\mathbf{S}}_{j,0}$ are the corresponding columns of any structured left-inverse $\widetilde{\mathbf{S}}$ of $\mathbf{R}_{\mathbf{b},a}$ as in (11.23). Note that $\mathbf{c}_j$ is nothing but the M-periodic sequence in $\ell^2_M(\mathbb{Z})$ derived from the column $\widetilde{\mathbf{S}}_{j,0} \in \mathbb{C}^M$ of $\widetilde{\mathbf{S}}$.

The dihedral group case

Let D_3 be the dihedral group $D_3 = \big\{e,\ g,\ g^2,\ k,\ kg,\ kg^2\big\}$ of the symmetries of the equilateral triangle, i.e., g is a rotation of $2\pi/3$ and k is the axial reflection. They satisfies the relationships $g^3 = k^2 = e$ and $kg = g^2k$. Consider its normal subgroup $H = \big\{e,\ g,\ g^2\big\}$; as a consequence, the quotient group $D_3/H = \{[e], [k]\}$, is a cyclic group of order 2, and $K = \{e, k\}$.

Let $s \in D_3 \mapsto U(s) \in \mathcal{U}(\mathcal{H})$ be a unitary representation of D_3 in a Hilbert space $\mathcal{H}$. Fixed $|a\rangle \in \mathcal{H}$ we consider $\mathcal{H}_a$ the subspace of $\mathcal{H}$ spanned by $\big\{U(s)a\ :\ s \in D_3\big\}$. In case this set is linearly independent in $\mathcal{H}$ it can be described as the unique expansion $|x\rangle = \sum_{s\in D_3} \alpha_s\, U(s)|a\rangle$, with $\alpha_s \in \mathbb{C}$.

Assume that N $\mathcal{L}_j$-systems, $j = 1, 2, \ldots, N$, are defined on $\mathcal{H}_a$. In this case, each 2×6 block $\mathbf{R}_{b_j,a}$ of the $2N \times 6$ matrix $\mathbf{R}_{\mathbf{b},a}$ in (11.13) is given by

$$\mathbf{R}_{b_j,a} = \begin{pmatrix} R_{b_j,a}(e) & R_{b_j,a}(g) & R_{b_j,a}(g^2) & R_{b_j,a}(k) & R_{b_j,a}(kg) & R_{b_j,a}(kg^2) \\ R_{b_j,a}(k) & R_{b_j,a}(kg) & R_{b_j,a}(kg^2) & R_{b_j,a}(e) & R_{b_j,a}(g) & R_{b_j,a}(g^2) \end{pmatrix}$$

If rank $\mathbf{R}_{\mathbf{b},a} = 6$, then, according to Theorem 1 there exist N vectors $|c_j\rangle \in \mathcal{H}_a$, $j = 1, 2, \ldots, N$, such that the sequence $\big\{U(s)|c_j\rangle\big\}$, $j = 1, 2, \ldots, N$, $s \in \{e, k\}$ is a frame for $\mathcal{H}_a$ and, for any $|x\rangle \in \mathcal{H}_a$ the sampling expansion

$$|x\rangle = \sum_{j=1}^{N} \sum_{s\in\{e,k\}} \mathcal{L}_j x(s)\, U(s)|c_j\rangle\,,$$

holds. Moreover, $|c_j\rangle = \mathcal{T}_a^{D_3}(\widetilde{\mathbf{S}}_{j,e})$, $j = 1, 2, \ldots, N$, where $\widetilde{\mathbf{S}}_{j,e}$ denotes the corresponding column of any $6 \times 2N$ left-inverse $\widetilde{\mathbf{S}}$ of $\mathbf{R}_{\mathbf{b},a}$ as in (11.23). A similar result applies for the general dihedral group D_m.

11.5 Discussion and Conclusions

A sampling expansion for a vector state $|x\rangle$ in an invariant subspace $\mathcal{H}_a$ of a Hilbert space $\mathcal{H}$ with respect a unitary representation $U(g)$ of a given finite group G has been obtained. The generalized samples are obtained by convolution in the auxiliary Hilbert space $L^2(G)$, of the the fundamental cross-covariance matrix $\mathbf{R}_{\mathbf{b},a}$ of the finite sequence of vectors $U(k_n)|b_j\rangle$ with the original state. The reconstruction is achieved as a linear superposition of a finite frame $\{|C_{j,n}\rangle\}$ with these coefficients. The elements $|C_{j,n}\rangle$ of the frame are compatible with the unitary structure of the problem in the sense that they have the form $|C_{j,n}\rangle = U(k_n)|c_j\rangle$ for some elements $|c_j\rangle$ in $\mathcal{H}_a$ and they are constructed in a natural way from a left-inverse of the fundamental cross-covariance matrix.

The sampling expansions obtained would allow for a reconstruction of the original state, as well as its unitary evolution if the group G is a symmetry of the dynamics, using frames adapted to the structure of the problem, that is, a family of states which, in general, do not form an orthonormal basis of the system and prepared independently of the initial state by using the geometry of the group G. The determination of the samples by means of generalized measurements on the auxiliary Hilbert space $L^2(G)$ and the reconstruction of the unitary evolution will be discussed in subsequent works.

The use of frames adapted to the geometry of the group G and an Abelian subgroup H as discussed in this paper, could be relevant in solving such relevant problem as Kitaev's Abelian stabilizer problem or designing faster phase estimation quantum algorithms [22].

Molecular symmetry theory will constitute another obvious applications of the theory as it would provide a new way of representing molecular states by using frames and generalized samples. Such issues will be considered in future publications.

The results obtained in this paper for finite groups have natural extensions to compact and type I discrete groups. Other groups of physical relevance like the Heisenberg-Weyl group and other nilpotent and solvable groups will be discussed elsewhere.

Acknowledgements The authors acknowledge financial support from the Spanish Ministry of Economy and Competitiveness, through the Severo Ochoa Programme for Centres of Excellence in RD (SEV-2015/0554). AI would like to thank partial support provided by the MINECO research project MTM2017-84098-P and QUITEMAD+, S2013/ICE-2801.

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Chapter 12
On the Kinematics of the Last Wigner Particle

José M. Gracia-Bondía and Joseph C. Várilly

Abstract Wigner's particle classification provides for 'continuous spin' representations of the Poincaré group, corresponding to a class of (as yet unobserved) massless particles. Rather than building their induced realizations by use of "Wigner rotations" in the textbooks' way, here we exhibit a scalar-like first-quantized form of those (bosonic) Wigner particles directly, by combining wave equations proposed by Wigner long ago with a recent prequantized treatment employing Poisson structures.

12.1 Introduction

By the last Wigner particle (WP) here is meant the last case in Wigner's classification of unirreps of the Poincaré group [1]: massless particles whose second Casimir has a nonzero value. More often, they are referred to as continuous spin particles (CSP) – somewhat of a misnomer. Though routinely dismissed as "unobserved" in standard textbook treatments, the possible existence and properties of such particles are of continued interest [2]; after pioneering work by Schuster and Toro [3–5], several recent studies [6–10] have appeared. Closer to the spirit of this paper is the construction by Rehren [11] stemming from his own work with Mund and Schroer – see [12] and references therein – of a string-local quantum field for such a particle, as a "Pauli–Lubański limit" of massive, string-local fields. At an opposite end, mathematically speaking, our own construction [13] of a "classical elementary system" for the WP foreshadows its quantum kinematics.

Our goal here is to review the first-quantized description of the (bosonic) WP: this is the relevant approach for certain applications that do not require a full-blown

J. M. Gracia-Bondía (✉)
Escuela de Física, Universidad de Costa Rica, San José 11501, Costa Rica

Departamento de Física Teórica, Universidad de Zaragoza, 50009 Zaragoza, Spain
e-mail: jmgb@unizar.es

J. C. Várilly
Escuela de Matemática, Universidad de Costa Rica, San José 11501, Costa Rica
e-mail: joseph.varilly@ucr.ac.cr

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_12

quantum field formalism. In principle, such a description is already available, by means of little-group techniques [14, 15]. However, one can attain a simpler-looking scalar-like version by starting directly from the wave equations. Among our purposes here is to delineate this version, less cumbersome than the standard approach.

The plan of the article is as follows. In Sect. 12.2 we recall the theory of the second Casimir associated to the Poincaré group, borrowing a method and notation going back to work by Schwinger [16]. We also bring in a quite instrumental result on the Wigner rotation for massless particles [17]. Section 12.3 is the core of the paper. There we introduce an appropriate set of states for the WP, and we show the invariant nature of their associated wavefunctions, their equations of motion, and the existence of an invariant scalar product. In Sect. 12.4 we exhibit the causal propagator for the boson WP. Section 12.5 deals briefly with the relation between the invariant and the conventional formalisms.

In the appendices we state and develop our Poincaré-group conventions, and then expound a relevant aspect of little-group theory that we have not found in the standard presentations.

12.2 The Schwinger Decomposition of the Pauli–Lubański Operator

Before coming to the (one-particle) Hilbert space for the WP, let us recall the standard basis of the Lie algebra $\mathfrak{p}$ of the Poincaré group $\mathcal{P}_+^\uparrow$ whose 10 generators $\{P^0, P^a, L^a, K^a : a = 1, 2, 3\}$ correspond respectively to time translation, space translations, rotations and boosts – consult Appendix 1 for our notation and conventions. The commutation relations for the Lorentz subgroup are as follows:

$$[L^a, L^b] = \varepsilon^{ab}{}_c\, L^c, \qquad [L^a, K^b] = \varepsilon^{ab}{}_c\, K^c, \qquad [K^a, K^b] = -\varepsilon^{ab}{}_c\, L^c.$$

The pseudovector operator (in the enveloping algebra of $\mathfrak{p}$)

$$\begin{aligned} W^\rho &:= J^{*\rho\mu} P_\mu = P_\mu J^{*\rho\mu} = (\boldsymbol{P}\cdot\boldsymbol{L},\ P^0\boldsymbol{L} + \boldsymbol{K}\times\boldsymbol{P}) \equiv (W^0, \boldsymbol{W}) \\ &= \big(P^1 J^{23} + P^2 J^{31} + P^3 J^{12},\ P^0 J^{23} + P^2 J^{30} + P^3 J^{02}, \\ &\quad P^0 J^{31} + P^1 J^{03} + P^3 J^{10},\ P^0 J^{12} + P^2 J^{10} + P^1 J^{02}\big) \end{aligned} \tag{12.1}$$

is referred to as the *Pauli–Lubański vector*. It clearly satisfies

$$(WP) = 0 \quad \text{and} \quad [P^\nu, W^\mu] = 0,$$

and is a vector under the action of the Lorentz group generators:

$$[J^{\mu\nu}, W^\tau] = g^{\tau\nu} W^\mu - g^{\tau\mu} W^\nu.$$

As a corollary, one obtains the identities:

$$[W^\mu, W^\nu] = \varepsilon^{\mu\nu}{}_{\tau\rho} W^\tau P^\rho; \quad \text{and} \quad [J^{\mu\nu}, (WW)] = 0; \tag{12.2}$$

the second one indicating that (WW) is a Casimir operator for $\mathcal{P}_+^\uparrow$. One finds also that

$$(WW) = \tfrac{1}{4}\varepsilon^{\rho\mu\nu\tau} P_\mu J_{\nu\tau}\, \varepsilon_{\rho\kappa\sigma\eta} P^\kappa J^{\sigma\eta} = -\tfrac{1}{2} J_{\nu\tau} J^{\nu\tau} P^2 + J_{\kappa\sigma} J^{\mu\sigma} P^\kappa P_\mu\,. \tag{12.3}$$

We assume in what follows that $P^0 > 0$. By invoking expression (12.1) in the rest frame, it becomes clear that the Casimir (WW) for a massive particle equals $-m^2 \boldsymbol{S}\cdot\boldsymbol{S}$, where $\boldsymbol{S}$ is the spin generator. This tells us that (WW) captures *internal* angular momentum. In general W is spacelike,[1] except that in the massless case it can be parallel to P: this leads to the known fixed-helicity particles, like the photon and graviton, for which relations (12.2) are trivial.

Here we put that case aside: the Wigner particle *by definition* obeys

$$(WW) = -\kappa^2 < 0.$$

We have seen in (12.1) that the temporal component of W is directly related to helicity, which deserves a symbol:

$$H := (\boldsymbol{P}\cdot\boldsymbol{L})/P^0. \quad \text{Therefore} \quad W^0 = H P^0. \tag{12.4}$$

The relation $(WP) = 0$ implies that the relevant part of $\boldsymbol{W}$ is that which is transverse to $\boldsymbol{P}$:

$$\boldsymbol{T} := \boldsymbol{W} - W^0 \boldsymbol{P}/P^0 = \boldsymbol{W} - (\boldsymbol{W}\cdot\boldsymbol{P})\boldsymbol{P}/(P^0)^2, \quad \text{so that} \quad \boldsymbol{W} = H\boldsymbol{P} + \boldsymbol{T}. \tag{12.5}$$

Notice that $\boldsymbol{T}^2 = \kappa^2$. We call $\boldsymbol{W} = H\boldsymbol{P} + \boldsymbol{T}$ the Schwinger decomposition of (the spatial part of) the PL vector; the notation $\boldsymbol{T}$ for the part of $\boldsymbol{W}$ transverse to $\boldsymbol{P}$ follows [16]. Not only do the components of $\boldsymbol{T}$ commute with the momentum; they commute with each other. This is worth a proof:

$$\begin{aligned}
[T^a, T^b] &= [W^a, W^b] - [W^0, W^b]P^a/P^0 - [W^a, W^0]P^b/P^0 \\
&= \varepsilon^{ab}{}_c T^c P^0 - \varepsilon^b{}_{de} T^d P^e P^a/P^0 + \varepsilon^a{}_{rs} T^r P^s P^b/P^0 \\
&= \varepsilon^{ab}{}_c T^c P^0 - (\boldsymbol{T}\times\boldsymbol{P})^b P^a/P^0 + (\boldsymbol{T}\times\boldsymbol{P})^a P^b/P^0 \\
&= \varepsilon^{ab}{}_c \big(T^c P^0 + ((\boldsymbol{T}\times\boldsymbol{P})\times\boldsymbol{P})^c/P^0\big) = \varepsilon^{ab}{}_c \big(T^c P^0 - T^c (P^0)^2/P^0\big) = 0.
\end{aligned}$$

Schwinger writes for this: $\boldsymbol{T}\times\boldsymbol{T} = \boldsymbol{0}$. Note also that

$$[H, K^a] = T^a/P^0; \qquad [K^a, T^b] = T^a P^b/P^0.$$

[1] Since $(WP) = 0$ and $(PP) \geq 0$ together imply that $(WW) \leq 0$.

Let us introduce another spatial 3-vector, also transverse to $\boldsymbol{P}$:

$$\boldsymbol{Y} := (\boldsymbol{P}/P^0) \times \boldsymbol{T}.$$

There is a 4-vector naturally associated with $\boldsymbol{Y}$ like W with $\boldsymbol{T}$. But we do not go into that. Note the commutator relation

$$[H, T^a] = [W^0, T^a]/P^0 = \varepsilon^a{}_{bc} T^b P^c/P^0 = \boldsymbol{T} \times \boldsymbol{P}^a/P^0 = -Y^a,$$

which is at once accompanied by

$$\begin{aligned}[H, Y^a] &= \varepsilon^a{}_{bc}[H, P^b T^c/P^0] = -\varepsilon^a{}_{bc} P^b Y^c/P^0 \\ &= -(\boldsymbol{P} \times \boldsymbol{Y})^a/P^0 = (\boldsymbol{P} \times (\boldsymbol{T} \times \boldsymbol{P}))^a (P^0)^{-2} = T^a.\end{aligned}$$

At this point, following Schwinger anew, and also inspired by [18], we may introduce a position vector commuting with H:

$$\boldsymbol{R} = -\tfrac{1}{2}[\boldsymbol{K}, (P^0)^{-1}]_+ - (\boldsymbol{T} \times \boldsymbol{P})(P^0)^{-3}.$$

Notice that

$$[W^0, \boldsymbol{R}] = -\frac{\boldsymbol{W}_\parallel}{P^0}, \quad \text{so} \quad [H, \boldsymbol{R}] = [W^0/P^0, \boldsymbol{R}] = -\frac{\boldsymbol{W}_\parallel}{(P^0)^2} + \frac{W^0 \boldsymbol{P}/P^0}{(P^0)^2} = 0.$$

We remark that $[P^j, R^k] = -\delta^{jk}$. Also, $[R^j, P^0] = P^j/P^0$ and $[R^j, (P^0)^{-1}] = -P^j/(P^0)^3$.

We list here some commutators involving $\boldsymbol{R}$:

$$\begin{aligned}&[R^j, P^k] = \delta^{jk}, \quad [R^j, P^0] = P^j (P^0)^{-1}, \qquad [W^0, R^j] = (T^j - W^j)(P^0)^{-1}, \\ &[R^j, H] = 0, \qquad [R^j, T^k] = -T^j P^k (P^0)^{-2}, \quad [R^j, R^k] = -\varepsilon_l^{jk} H P^l (P^0)^{-3}, \\ &[R^j, (\boldsymbol{T} \times \boldsymbol{P})^k (P^0)^{-2}] + [(\boldsymbol{T} \times \boldsymbol{P})^j (P^0)^{-2}, R^k] = 0. \end{aligned} \tag{12.6}$$

The sixth relation in (12.6) shows the WP to be intrinsically non-localizable. The proofs of the above are routine; and anyway, the Poisson brackets and general results of the thorough study of the kinematics of the WP in Kirillov's prequantized formalism [13] can be largely transposed here. In particular: the commuting orthogonal trihedron $(\boldsymbol{P}, \boldsymbol{T}, \boldsymbol{Y})$ *rotates gyroscopically* under boosts, this being *ipso facto* true for all (restricted) Lorentz transformations. While the length of $\boldsymbol{P}$ can vary, the lengths of $\boldsymbol{T}$ and $\boldsymbol{Y}$ are fixed at κ. The next subsection helps to understand why.

12.2.1 The Wigner Rotation, Tamed

In the massive case there is a canonical definition for a Lorentz transformation taking the reference momentum $(m, \mathbf{0})$ to p, as a boost $L_{\zeta \boldsymbol{n}}$ with direction $\boldsymbol{n}$ (a unit vector) and boost parameter ζ. The corresponding Wigner rotation acting[2] on a 3-vector $\boldsymbol{v}$ is found in [13, 17]:

$$R(L_{\zeta \boldsymbol{n}}, p)\boldsymbol{v} = R_{\boldsymbol{m},\delta}\boldsymbol{v} = \boldsymbol{v}\cos\delta + \boldsymbol{m}\times\boldsymbol{v}\sin\delta + (\boldsymbol{m}\cdot\boldsymbol{v})\boldsymbol{m}(1-\cos\delta),$$

where:

$$\boldsymbol{m} = \frac{\boldsymbol{p}\times\boldsymbol{n}}{|\boldsymbol{p}\times\boldsymbol{n}|};\quad \cos\delta = 1 - \frac{|\boldsymbol{p}\times\boldsymbol{n}|^2(\cosh\zeta - 1)}{(m+p^0)(m+p'^0)},$$
$$\sin\delta = \frac{(m+p^0)\sinh\zeta + \boldsymbol{n}\cdot\boldsymbol{p}(\cosh\zeta-1)}{(m+p^0)(m+p'^0)}\,|\boldsymbol{p}\times\boldsymbol{n}|,$$

with the action $p \mapsto p'$ on 4-momenta given by:

$$p'^0 = p^0\cosh\zeta + \boldsymbol{n}\cdot\boldsymbol{p}\sinh\zeta,$$
$$\boldsymbol{p}' = \boldsymbol{p} + p^0\boldsymbol{n}\sinh\zeta + (\boldsymbol{n}\cdot\boldsymbol{p})\boldsymbol{n}(\cosh\zeta - 1).$$

As remarked in [17], the massless limit of $\sin\delta$ is perfectly smooth:

$$\sin\delta = \left(\frac{\sinh\zeta}{p'^0} + \frac{\boldsymbol{n}\cdot\boldsymbol{p}(\cosh\zeta-1)}{p^0p'^0}\right)|\boldsymbol{p}\times\boldsymbol{n}|, \tag{12.7}$$

whereas

$$\boldsymbol{p}\times\boldsymbol{p}' = \left[p^0\sinh\zeta + \boldsymbol{n}\cdot\boldsymbol{p}(\cosh\zeta-1)\right]\boldsymbol{p}\times\boldsymbol{n};$$

therefore the component of $\boldsymbol{p}'$ not along $\boldsymbol{p}$ stays in the plane perpendicular to $\boldsymbol{p}\times\boldsymbol{n}$. The sine of the angle of rotation is given by

$$\frac{|\boldsymbol{p}\times\boldsymbol{p}'|}{|\boldsymbol{p}||\boldsymbol{p}'|} = \frac{p^0\sinh\zeta + \boldsymbol{n}\cdot\boldsymbol{p}(\cosh\zeta-1)}{|\boldsymbol{p}||\boldsymbol{p}'|}\,|\boldsymbol{p}\times\boldsymbol{n}|. \tag{12.8}$$

In the massive case (where $p^0p'^0 > |\boldsymbol{p}||\boldsymbol{p}'|$), this angle is generally greater than the Wigner rotation angle δ. The key point is that this formula makes perfect sense for $m = 0$, even though some of the factors in its definition do not. Namely, keeping in mind that in the massless case $p^0 = |\boldsymbol{p}|$ and $p'^0 = |\boldsymbol{p}'|$, the formula (12.8) exactly matches formula (12.7). Which means that momentum and "spin" turn in solidarity. Wigner graphically describes why in the massless case they must do so: "for a

[2] In the "active transformation" view [19, Sect. 3.3].

particle with zero rest-mass [...] if we connect any internal motion with the spin, this is perpendicular to the velocity" [20].

12.3 The Invariant Formalism for the WP

To construct a Hilbert space $\mathcal{H}$ carrying a unitary irreducible representation (or "unirrep") U of the Poincaré group $\mathcal{P}_+^\uparrow$ corresponding to a Wigner particle with Casimir κ^2, we proceed by taking a basic set of kets, labelled as $\big||\boldsymbol{p}|,\, \boldsymbol{p}/|\boldsymbol{p}|,\, \boldsymbol{t}\big\rangle$; where[3]

$$\mathbb{P}^\mu\, |\boldsymbol{p}, \boldsymbol{t}\rangle = \mathbb{P}^\mu \big||\boldsymbol{p}|,\, \boldsymbol{p}/|\boldsymbol{p}|,\, \boldsymbol{t}\big\rangle = p^\mu\, \big||\boldsymbol{p}|,\, \boldsymbol{p}/|\boldsymbol{p}|,\, \boldsymbol{t}\big\rangle,$$
$$\mathbb{T}\big||\boldsymbol{p}|,\, \boldsymbol{p}/|\boldsymbol{p}|,\, \boldsymbol{t}\big\rangle = \boldsymbol{t}\, \big||\boldsymbol{p}|,\, \boldsymbol{p}/|\boldsymbol{p}|,\, \boldsymbol{t}\big\rangle.$$

Here $\mathbb{P}^\mu$ is the selfadjoint operator corresponding to the generator P^μ; $\mathbb{T}$ is the 3-component selfadjoint operator corresponding to Schwinger's geometric generator $\boldsymbol{T}$; and $\boldsymbol{t}$ is the 3-vector of its eigenvalues. These polarization states lie on a circle of radius κ in the plane perpendicular to $\boldsymbol{p}$. Thus, with some abuse of notation, we can rewrite $|\boldsymbol{p}, \theta\rangle$ or $|\kappa;\, \boldsymbol{p}, \theta\rangle$ for those kets, with θ denoting their angular degree of freedom. Note that different positive values of κ correspond to inequivalent representations of $\mathcal{P}_+^\uparrow$.

The gyroscopic property is the key to the strange simplicity of the WP structure, as it indicates that the corresponding wave-functions for the WP may transform similarly to spin-zero particles. Indeed, for *any* Lorentz transformation Λ the gyroscopic property implies that the rotation $R_\Lambda\colon \boldsymbol{p}/|\boldsymbol{p}| \mapsto \boldsymbol{p}'/|\boldsymbol{p}'|$ applies equally to $\boldsymbol{t}$, i.e., $\boldsymbol{t} \mapsto \boldsymbol{t}' = R_\Lambda \boldsymbol{t}$. This is clear if Λ is a rotation, and has been shown in [13] when Λ is a boost; and so it is true of any Λ.

Remark 1 The little-group techniques demand the choice of a Lorentz transformation at each point of (the mantle of) the lightcone. Now, it is not possible, for rather obvious topological reasons [21], to construct a global continuous section of the $SL(2, \mathbb{C})$-principal bundle. Since one works mostly in the category of Hilbert spaces, and there *exist* Borel sections, this is usually deemed not too serious a problem. However, it does produce some pathologies, which, according to the analysis in [22], for ordinary massless particles of nonzero helicity at least, partially invalidate the concept of sharp momentum states that people have been using all along. It seems unlikely that related troubles manifest themselves for WPs in the invariant formulation. On the other hand, the very fact that the description of one of their states requires three angles, instead of two, makes for more singular eigenstates than for scalar particles.

It pertains to declare the normalization of our kets. We decide for the Lorentz-invariant expression:

[3] We use open-faced type for the operators on Hilbert space corresponding to geometrical generators.

$$\langle \boldsymbol{p}, \boldsymbol{t} \mid \boldsymbol{p}', \boldsymbol{t}' \rangle = |\boldsymbol{p}|\, \delta(\boldsymbol{p} - \boldsymbol{p}')\, \delta(\boldsymbol{t} - \boldsymbol{t}'), \quad \text{or}$$
$$\langle \boldsymbol{p}, \theta \mid \boldsymbol{p}', \theta' \rangle = |\boldsymbol{p}|\, \delta(\boldsymbol{p} - \boldsymbol{p}')\, \delta(\theta - \theta').$$

Let $\Phi(\boldsymbol{p}, \theta) := \langle \boldsymbol{p}, \theta \mid \Phi \rangle$. An inner product for these wavefunctions is thus given by

$$\langle \Phi \mid \Phi \rangle \propto \int \frac{d^3 p}{|\boldsymbol{p}|}\, d\theta \left| \Phi(\boldsymbol{p}, \theta) \right|^2. \tag{12.9}$$

The definition does not depend on the Lorentz frame [23]. We give an explicitly invariant form of $\langle \Phi \mid \Phi \rangle$ in momentum space at the end of this section; and also a formula in configuration space. In order to see them, and to better grasp the kinematics of the WP, we introduce, following Wigner, its manifestly invariant formalism.

12.3.1 Equations of Motion

As advertised, the gyroscopic property implies that equations of motion for the WP may be of scalar-like form. In fact, Wigner returned many times [23–25] to the question of equations of motion for a WP. In those papers Wigner considers scalar wave functions depending on configuration or momentum-space variables and an extra spacelike 4-vector variable,[4] transforming covariantly under the Lorentz group, and satisfying the equations:

$$\Box_x \Phi(x, w) = 0; \quad \text{or} \quad p^2\, \Phi(p, w) = 0, \tag{12.10a}$$
$$(w^2 + \kappa^2)\, \Phi(x, w) = 0; \quad \text{or} \quad (w^2 + \kappa^2)\, \Phi(p, w) = 0, \tag{12.10b}$$
$$(w\, \partial_x)\, \Phi(x, w) = 0; \quad \text{or} \quad (pw)\, \Phi(p, w) = 0, \tag{12.10c}$$
$$\big((\partial_x \partial_w) + 1\big) \Phi(x, w) = 0; \quad \text{or} \quad \big((p\, \partial_w) + i\big) \Phi(p, w) = 0. \tag{12.10d}$$

The first three equations have a ready interpretation, corresponding respectively to the Klein–Gordon equation for a massless particle, the value of the second Casimir associated to a given WP, and mutual perpendicularity of the momentum and PL vectors.

For the fourth equation, just note that identifying the equations of motion with the action of the Casimir operators is a matter of principle. So let us formally take P and W as independent variables at the same title, in a representation in which P is diagonal, and compute from equation (12.3) with $P^2 = 0$ the second Casimir:

[4] Here called w, since it will be seen to be an avatar of the PL vector.

$$
\begin{aligned}
C_2 \equiv (WW) &= (w_\nu\, \partial_\rho^w - w_\rho\, \partial_\nu^w)(w^\nu\, \partial_w^\sigma - w^\sigma\, \partial_w^\nu)\, \partial_\sigma^x\, \partial_x^\rho \\
&= -\kappa^2 (\partial_x \partial_w)^2 + (w\,\partial_x)(\partial_x \partial_w) - (w\,\partial_x)(w\,\partial_w)(\partial_x \partial_w) - (w\,\partial_w)\Box_x \\
&\quad - (w\,\partial_x)(w\,\partial_w)(\partial_x \partial_w) - 4(w\,\partial_x)(\partial_x \partial_w) + (w\,\partial_x)^2\,\Box_w + (w\,\partial_x)(\partial_w \partial_x) \\
&= -\kappa^2 (\partial_x \partial_w)^2 + (w\,\partial_x)^2\,\Box_w - 2(w\,\partial_x)(\partial_x \partial_w)(w\,\partial_w) - (w\,\partial_w)\Box_x \\
&= \kappa^2 (p\,\partial_w)^2 - (pw)^2\,\Box_w + 2(pw)(p\,\partial_w)(w\,\partial_w) = -\kappa^2. \qquad (12.11)
\end{aligned}
$$

Now, since here $(pw) = 0$, we are left with $(\partial_x \partial_w) = \mp 1$, which arguably completes the Wigner equations (12.10) above.[5]

The weak point of the argument appears to be that the components of W do not commute in general. But the equations defend themselves very well: the last one is immediately integrated,

$$\Phi(\boldsymbol{p}, w - \gamma p) = e^{\pm i\gamma}\, \Phi(\boldsymbol{p}, w), \qquad (12.12)$$

and may be interpreted as an infinitesimal gauge transformation, which, in view of the Schwinger decomposition (12.4) and (12.5), identifies γ as the placeholder for helicity. One recognizes that the argument w in (12.10) stands for both "spin" and "gauge" degrees of freedom.

The Wigner system of equations is consistent; indeed, compatibility between the third and fourth equations is guaranteed precisely by the wave equation (12.10a), and compatibility between the second and fourth by the third equation (12.10c). That is to say: the differential operators in the left column of (12.10) form a closed system, since $\Box_x$ commutes with the other three, which have the nontrivial commutation relations:

$$[(\partial_x \partial_w) + 1, w^2 + \kappa^2] = 2(w\,\partial_x), \quad [(w\,\partial_x), (\partial_x \partial_w) + 1] = \Box_x\,.$$

This would not hold were $m > 0$, requiring $\Box_x + m^2$ in (12.10a). Moreover, were $\kappa = 0$, then (12.10d) would not follow from (12.11). What is more: in the light of the display above, the two key equations are (12.10d) and (12.10b), since we may regard the other two – whose physical meaning is obvious – as their compatibility conditions. In summary: the system (12.10) is associated specifically to the WP.

Let us consider the transformation $\partial_w \mapsto i v$, $w \mapsto -i\,\partial_v$ in the Wigner system of equations [26, 27]. There ensues the relation

$$
\begin{aligned}
(WW) &= 2(pw)(p\,\partial_w)(w\,\partial_w) - w^2 (p\,\partial_w)^2 - (pw)^2\,\Box_w \\
&= 2(pv)(p\,\partial_v)(v\,\partial_v) - v^2 (p\,\partial_v)^2 - (pv)^2\,\Box_v.
\end{aligned}
$$

Therefore (WW) is Fourier-invariant in this sense.

[5] For definiteness, we opted for the upper sign in (12.10d); taking the lower one amounts to changing the sign of κ only.

In terms of this Fourier-conjugate to w, we now obtain the "smooth solutions" by Schuster and Toro [3]:

$$(p\partial_v)\widetilde{\Phi}(\boldsymbol{p}, v) = 0.$$

Also, the equations in [11] coincide essentially with those of [3].[6] The associated action functionals [5, 28, 29] look quite complicated.

12.3.2 Invariant Wavefunctions

The Wigner equation (12.10a) tells us that we are on-shell in momentum. We express this by

$$\Phi(x, w) \propto \int d^4p\, \theta(p^0)\, \delta(p^2) e^{-i(px)} \Phi(\boldsymbol{p}, w) \propto \int \frac{d^3\boldsymbol{p}}{|\boldsymbol{p}|}\, e^{-i(px)} \Phi(\boldsymbol{p}, w),$$

and equivalently

$$\Phi(\boldsymbol{p}, w) \propto \int d^4x\, e^{i(px)}\, \Phi(x, w)\Big|_{p^0=|\boldsymbol{p}|},$$

with our choice of sign for p^0. Now we may relate the above $\langle \boldsymbol{p}, \boldsymbol{t} \mid \Phi\rangle$ with $\Phi(x, w)$. Consider again (12.10d), or formula (12.12), and let the gauge $\gamma := w^0/p^0 = w^0/|\boldsymbol{p}|$. It follows that

$$\begin{aligned}\Phi(\boldsymbol{p}, w) &\equiv \Phi(\boldsymbol{p}, w^0, \boldsymbol{w}_\parallel, \boldsymbol{t}) = \exp(-i w^0/|\boldsymbol{p}|)\, \Phi(\boldsymbol{p}, 0, \boldsymbol{t}) \\ &=: \exp(-i w^0/|\boldsymbol{p}|)\, \langle \boldsymbol{p}, \boldsymbol{t} \mid \Phi\rangle = \exp(-i\, \boldsymbol{p}\cdot\boldsymbol{w}/|\boldsymbol{p}|^2)\, \langle \boldsymbol{p}, \boldsymbol{t} \mid \Phi\rangle \\ &=: \exp(-i(\boldsymbol{p}\cdot\boldsymbol{w})/|\boldsymbol{p}|^2)\, \langle \boldsymbol{p}, \theta \mid \Phi\rangle.\end{aligned}$$

For any $(\boldsymbol{p}, \theta)$ there holds $|\Phi(\boldsymbol{p}, \gamma, \theta)| = |\Phi(\boldsymbol{p}, 0, \theta)|$. Notice that for the definition (12.9) of the scalar product one should not integrate on the real gauge variable γ, which would yield a divergent expression.

The corresponding representation U of $\mathcal{P}_+^\uparrow$ satisfies

$$U(a, \Lambda)\, \Phi(x, w) = \Phi\big(\Lambda^{-1}(x - a), \Lambda^{-1} w\big)$$

on the space of solutions of the (12.10). We have found the simple theory of an invariant object for the WP – with the help of the Wigner equations themselves.

The internal parts of Lorentz group generators in this formalism commute with the orbital parts. They are of the form [23]:

[6] "... alle diese Gleichungssysteme, sofern sie widerspruchsfrei sind, äquivalent sind" [24].

$$\mathbb{K}^c_{\text{int,cov}} = i\big(w^0\partial_{w^c} + w^c\partial_{w^0}\big) =: \mathbb{K}^c_w;$$
$$\mathbb{L}^c_{\text{int,cov}} = -i\,\varepsilon^c{}_{ab}\,w^a\partial_{w^b} =: \mathbb{L}^c_w \equiv \mathbb{S}^c.$$

Note the commutation relations $\mathbb{S}\times\mathbb{S} = i\mathbb{S}$, in Schwinger's notation; and that the total angular momentum generators can be written as $\mathbb{L} = -i\,\boldsymbol{p}\times\partial_{\boldsymbol{p}} + \mathbb{S}$, just like for massive particles.

Remark 2 Given p such that $p^2 = 0$ and $p^0 > 0$, its three-dimensional little group G_p of rotations around $\boldsymbol{p}/|\boldsymbol{p}|$ and *null rotations* preserving $\boldsymbol{p}$ is well known. Any proper, orthochronous Lorentz transformation of the sphere must have (properly counted) two fixed points [30]. One possibility is that both null directions *coincide*; these are precisely the parabolic Lorentz transformations, called in context "null rotations"; they are discussed further in Appendix 2.[7]

Given a pair (p, w) satisfying $p^0 > 0$, $p^2 = (pw) = w^2 + \kappa^2 = 0$ and another pair (p', w') of the same kind, there is a *unique* restricted Lorentz transformation Λ such $\Lambda p = p'$ and $\Lambda w = w'$.

Remark 3 The scalar product (12.9) is Lorentz-invariant, though not obviously so. A manifestly invariant form of the scalar product appears in Wigner [24]: given two solutions $\Phi(p, w)$, $\Psi(p, w)$ of (12.10), define $\langle\Psi \mid \Phi\rangle$ by:

$$2\int d^4p\,d^4w\;\Psi^*(p,w)\,\Phi(p,w)\,\delta(p^2)\,\delta(w^2+\kappa^2)\,\delta\big((pw)\big)\,(pu)\,\delta\big((uw)-a\big), \tag{12.13}$$

where u is *any* timelike 4-vector such that $u^2 = 1$ and a an arbitrary parameter. For the convenience of the reader we follow Wigner in verifying that the integral is independent of such u and a. Differentiating first with respect to a,

$$\begin{aligned}
&\frac{d}{da}\langle\Psi \mid \Phi\rangle \\
&= -2\int d^4p\,d^4w\;\Psi^*(p,w)\,\Phi(p,w)\,\delta(p^2)\,\delta(w^2+\kappa^2)\,\delta\big((pw)\big)\,(p\partial_w)\,\delta\big((uw)-a\big) \\
&= 2\int d^4p\,d^4w\;\Psi^*(p,w)\,\Phi(p,w)\,p^2\delta(p^2)\,\delta(w^2+\kappa^2)\,\delta'\big((pw)\big)\,\delta\big((uw)-a\big) = 0.
\end{aligned}$$

Thus one can as well drop a in the expression (12.13). Next, by application of the differential operators $u_\alpha\,\partial/\partial u_\beta \mp u_\beta\,\partial/\partial u_\alpha$, one easily checks that the same expression is independent of the direction of u. So we can as well choose $u = (1, \boldsymbol{0})$, leading to

[7] The most general transformation fixing a null direction decomposes into a null rotation (belonging to a two-parameter set), a rotation and a boost. The four of them together constitute a *Borel subgroup* of the Lorentz group; the last two have as invariant directions those of $\boldsymbol{k}$ and the antipodal $-\boldsymbol{k}$; the boost does not leave k itself invariant.

$$\langle \Psi \mid \Phi \rangle = 2 \int d^4 p\, d^3 \boldsymbol{w}\, \Psi^*(p, w)\, \Phi(p, w)\, p^0\, \delta(p^2)\, \delta\big(|\boldsymbol{w}|^2 - \kappa^2\big)\, \delta(\boldsymbol{p} \cdot \boldsymbol{w})$$
$$= \int d^3 \boldsymbol{p}\, d^3 \boldsymbol{w}\, \Psi^*(p, w)\, \Phi(p, w)\, \delta\big(|\boldsymbol{w}|^2 - \kappa^2\big)\, \delta(\boldsymbol{p} \cdot \boldsymbol{w}),$$

which, with $p^0 = |\boldsymbol{p}|$ and $w^0 = 0$ in the arguments of the wavefunctions understood, coincides with (12.9).

Wigner [24] discusses as well in great detail the passage to x-space, yielding several equivalent forms, among which an attractive one is given by:

$$\langle \Psi \mid \Phi \rangle = \int d^3 \boldsymbol{x}\, d^3 \boldsymbol{w}\, \partial_t \Psi^*(x, w)\, \partial_t \Phi(x, w)\, \delta\big(|\boldsymbol{w}|^2 - \kappa^2\big)\, \delta(\boldsymbol{x} \cdot \boldsymbol{w}).$$

12.4 The Propagator

In our notation, and with slightly different conventions, the following formula is found in [31, (3.15)]:

$$\widetilde{D}(x, x'; w^0, \boldsymbol{w}, w'^0, \boldsymbol{w}') = -\widetilde{D}(x', x; w^0, \boldsymbol{w}, w'^0, \boldsymbol{w}')$$
$$= \delta(w^2 + \kappa^2)\, \frac{1}{(2\pi)^3} \int d^3 \boldsymbol{p}\, \frac{\sin |\boldsymbol{p}|(t - t')}{|\boldsymbol{p}|}\, e^{i \boldsymbol{p} \cdot (\boldsymbol{x} - \boldsymbol{x}')}\, \delta(pw)$$
$$\times\, \delta^3\big(|\boldsymbol{p}|(\boldsymbol{w} - \boldsymbol{w}') - (w^0 - w'^0)\boldsymbol{p}\big)\, e^{i(w^0 - w'^0)/|\boldsymbol{p}|}.$$

The above $\widetilde{D}$ is a Lorentz invariant distribution, which satisfies the Wigner equations.

Consider the skewsymmetric form s given by

$$s(\Psi, \Phi) := \int d^3 x' \left[\Psi(x')\, \partial_{t'} \Phi(x') - \Phi(x')\, \partial_{t'} \Psi(x')\right]_{t' = \text{const}}.$$

If D denotes the ordinary Jordan–Pauli propagator for massless fields, the solution of the wave equation with Cauchy data $\Phi(t', \boldsymbol{x}')|_{t' = \text{const}}$ is given by $s\big(D(x, -), \Phi(-)\big)$.

Now it should be clear that

$$\int d^4 w'\, s\big(\widetilde{D}(x, -; w, w'), \Phi(-; w')\big)$$
$$= \frac{\delta(w^2 + \kappa^2)}{(2\pi)^3} \int d^3 \boldsymbol{w}'\, \delta^3(\boldsymbol{w} - \boldsymbol{w}')\, \Phi(x; \boldsymbol{w}', w_0)\, \delta(pw) = \Phi(x; w),$$

if Φ already satisfies the Wigner equations; and this expression *becomes* a solution in the general case – since $\widetilde{D}$ itself satisfies them. Therefore this $\widetilde{D}$ behaves like a reproducing kernel, exactly as the ordinary Jordan–Pauli propagator, which repro-

duces any solution of the KG equation, and produces one such from an arbitrary spacetime function.

Notice moreover that $\widetilde{D}$ is *causal*: $\widetilde{D} = 0$ when $(x - x')^2 < 0$. This does not contradict Yngvason's theorem [32] on the nonlocality of quantum fields associated to WPs, for, among other reasons, the wavefunctions depend on an extra variable.

12.5 Connecting with the Standard Formalism

The *point de départ* of the standard formalism for the Wigner modules is the choice of a reference 4-momentum $k = (|\boldsymbol{k}|, \boldsymbol{k})$, which for massless particles can only be arbitrary. Its "length" $|\boldsymbol{k}|$ is irrelevant, so here it is assumed equal to one. The time-honoured choice for the reference momentum is $k := (1, 0, 0, 1)$. The representation space of its corresponding little group for a boson WP is spanned by vectors lying on the circle $|\boldsymbol{\xi}|^2 := (\xi^1)^2 + (\xi^2)^2 = \kappa^2$: either

$$|\xi^1, \xi^2\rangle \equiv |\kappa; \tau\rangle, \quad \text{where} \quad \tau := \arctan(\xi^2/\xi^1),$$

or $|\kappa; h\rangle$, with h denoting the helicity, computed with respect to the reference momentum. For these kets:

$$\mathbb{T}_{1,2}\,|\xi^1, \xi^2\rangle \equiv \mathbb{W}^{1,2}\,|\xi^1, \xi^2\rangle = \xi^{1,2}\,|\xi^1, \xi^2\rangle;$$

and also:

$$\exp(i\beta\mathbb{W}^0)\,|\kappa; \tau\rangle = |\kappa; \tau - \beta\rangle, \quad \text{or} \quad \exp(i\beta\mathbb{W}^0)\,|\kappa; h\rangle = e^{i\beta h}\,|\kappa; h\rangle.$$

Then one can employ the *standard* wave functions:

$$\psi_{\mathrm{st}}(\boldsymbol{p}, \xi^1, \xi^2) := \langle \boldsymbol{p}, \xi^1, \xi^2 \mid \psi\rangle$$

defined on the lightcone and the internal circle by the customary lifting to a unirrep space of the Poincaré group.

For a general unit vector $\boldsymbol{k}$, the generators of rotations take the form

$$\mathbb{L}_{\boldsymbol{k}} = -i\,\boldsymbol{p} \times \partial_{\boldsymbol{p}} + \frac{\boldsymbol{p} \times (\boldsymbol{k} \times \boldsymbol{p})}{|\boldsymbol{p}|(|\boldsymbol{p}| + \boldsymbol{k} \cdot \boldsymbol{p})}\,\mathbb{S} \cdot \boldsymbol{k} + \frac{\boldsymbol{p}}{|\boldsymbol{p}|}\,\mathbb{S}_{\boldsymbol{\xi}} \cdot \boldsymbol{k} = -i\,\boldsymbol{p} \times \partial_{\boldsymbol{p}} + \frac{\boldsymbol{p} + |\boldsymbol{p}|\boldsymbol{k}}{|\boldsymbol{p}| + \boldsymbol{k} \cdot \boldsymbol{p}}\,\mathbb{S}_{\boldsymbol{\xi}} \cdot \boldsymbol{k} \tag{12.14}$$

where $\boldsymbol{\xi}$ is taken transversal to $\boldsymbol{k}$ of norm κ, and $\mathbb{S}_{\boldsymbol{\xi}} := -i\boldsymbol{\xi} \times \partial_{\boldsymbol{\xi}}$. For the boost generators, one finds:

$$\begin{aligned}\mathbb{K}_{\boldsymbol{k}} &= i|\boldsymbol{p}|\,\partial_{\boldsymbol{p}} - \frac{\boldsymbol{k}\times\boldsymbol{p}}{|\boldsymbol{p}|+\boldsymbol{k}\cdot\boldsymbol{p}}\,\mathbb{S}_{\boldsymbol{\xi}}\cdot\boldsymbol{k} + \frac{\boldsymbol{p}\cdot\boldsymbol{\xi}}{|\boldsymbol{p}|^2}\,\frac{\boldsymbol{p}+|\boldsymbol{p}|\boldsymbol{k}}{|\boldsymbol{p}|+\boldsymbol{k}\cdot\boldsymbol{p}} - \frac{\boldsymbol{\xi}}{|\boldsymbol{p}|} \\ &= i|\boldsymbol{p}|\,\partial_{\boldsymbol{p}} - \frac{\boldsymbol{k}\times\boldsymbol{p}}{|\boldsymbol{p}|+\boldsymbol{k}\cdot\boldsymbol{p}}\,\mathbb{S}_{\boldsymbol{\xi}}\cdot\boldsymbol{k} + \frac{\boldsymbol{p}}{|\boldsymbol{p}|^2}\times\left(\frac{\boldsymbol{p}+|\boldsymbol{p}|\boldsymbol{k}}{|\boldsymbol{p}|+\boldsymbol{k}\cdot\boldsymbol{p}}\times\boldsymbol{\xi}\right). \qquad (12.15)\end{aligned}$$

The generators are defined on a (dense) subspace of the Hilbert space consisting of twice-differentiable functions vanishing on a cylinder centered on the negative $\boldsymbol{k}$-axis, including the origin – keep in mind the analysis in [22]. When $\boldsymbol{k} = (0, 0, 1)$, one recovers from (12.14) and (12.15) the familiar expressions found by Lomont and Moses [33] long ago.

It stands to reason that wavefunctions pertaining to the standard routine must be related to the invariant wavefunctions of Sect. 12.3.2 by unitary transformations. Let

$$\alpha := \arccos(\boldsymbol{k}\cdot\boldsymbol{p}/|\boldsymbol{p}|) = \arctan\frac{|\boldsymbol{p}-(\boldsymbol{p}\cdot\boldsymbol{k})\boldsymbol{k}|}{\boldsymbol{p}\cdot\boldsymbol{k}}\,.$$

In [31] one finds the assertion that such unitary transformations essentially consist of a rotation representative:

$$\delta(|\boldsymbol{\xi}|^2-\kappa^2)\,\delta(\boldsymbol{\xi}\cdot\boldsymbol{k})\,\psi_0(\boldsymbol{p},\boldsymbol{\xi}) := e^{iw^0/|\boldsymbol{p}|}\exp\left(i\alpha\,\frac{\boldsymbol{k}\times\boldsymbol{p}}{|\boldsymbol{k}\times\boldsymbol{p}|}\cdot\mathbb{S}\right)\Phi(\boldsymbol{p},w)\Big|_{\boldsymbol{w}=\boldsymbol{\xi}+w^0\boldsymbol{p}/|\boldsymbol{p}|}\,.$$

Reciprocally, given $\boldsymbol{k}$:

$$\begin{aligned}&\Phi(\boldsymbol{p},w) \\ &\quad= e^{-iw^0/|\boldsymbol{p}|}\exp\left(-i\alpha\,\frac{\boldsymbol{k}\times\boldsymbol{p}}{|\boldsymbol{k}\times\boldsymbol{p}|}\cdot\mathbb{S}_{\boldsymbol{\xi}}\right)\delta(|\boldsymbol{\xi}|^2-\kappa^2)\,\delta(\boldsymbol{\xi}\cdot\boldsymbol{k})\,\psi_0(\boldsymbol{p},\xi)\Big|_{\boldsymbol{\xi}=\boldsymbol{w}-w^0\boldsymbol{p}/|\boldsymbol{p}|}.\end{aligned}$$

Let us simply denote

$$V := \exp\left(i\alpha\,\frac{\boldsymbol{k}\times\boldsymbol{p}}{|\boldsymbol{k}\times\boldsymbol{p}|}\cdot\mathbb{S}\right).$$

It is perfectly true that V "diagonalizes" the helicity operator:

$$V(\mathbb{S}\cdot\boldsymbol{p}/|\boldsymbol{p}|)V^\dagger = \mathbb{S}\cdot\boldsymbol{k}.$$

Straightforward albeit tedious calculations show that the correct internal angular momentum components transversal to $\boldsymbol{k}$ in (12.14) are recovered by this unitary transformation. (See also [34, 35].) Unfortunately, we cannot go into this matter here.

Acknowledgements A report by Alejandro Jenkins of a conversation with Mark Wise set this work in motion. We are grateful to Alejandro, as well as to Fedele Lizzi and Patrizia Vitale, for discussions on the gyroscope property, and to Karl-Henning Rehren for most useful remarks about the equations by Wigner. We thank Daniel Solís for checking App. B and a useful observation. The project has received funding from the European Union's Horizon 2020 research and innovation programme

under the Marie Skłodowska-Curie grant agreement No. 690575. JMG-B received funding from Project FPA2015–65745–P of MINECO/Feder, and acknowledges the support of the COST action QSPACE. JCV received support from the Vicerrectoría de Investigación of the Universidad de Costa Rica.

Appendix 1: Poincaré Group Conventions

Our metric on the Minkowski space $\mathbb{M}$ is mostly-negative. The inner product of two vectors $x \equiv x^\mu$, $p \equiv p^\nu$ of spacetime is denoted with parentheses: $(xp) = x^\mu p_\mu$. When (we hope) it does not cause confusion, we often write $p^2 = (pp)$, say.

The Lie algebra $\mathfrak{p}$ of $\mathcal{P}$ has a basis of ten elements $\{P^0, P^a, L^a, K^a : a = 1, 2, 3\}$, corresponding respectively to time translations, space translations, rotations and boosts. The commutation relations for the Lorentz subgroup are as follows:

$$[L^a, L^b] = \varepsilon^{ab}{}_c\, L^c, \qquad [L^a, K^b] = \varepsilon^{ab}{}_c\, K^c, \qquad [K^a, K^b] = -\varepsilon^{ab}{}_c\, L^c.$$

The commutation relations are realized [8] by $K^a = \frac{1}{2}\sigma^a$ and $L^a = -\frac{i}{2}\sigma^a$.

In the real four-dimensional representation:

$$J^{01} \equiv K^1 = \begin{pmatrix} & 1 & & \\ 1 & & & \\ & & 0 & \\ & & & 0 \end{pmatrix}; \quad J^{02} \equiv K^2 = \begin{pmatrix} & & 1 & \\ & 0 & & \\ 1 & & & \\ & & & 0 \end{pmatrix}; \quad J^{03} \equiv K^3 = \begin{pmatrix} & & & 1 \\ & & 0 & \\ & 0 & & \\ 1 & & & \end{pmatrix};$$

$$J^{23} \equiv L^1 = \begin{pmatrix} 0 & & & \\ & 0 & & \\ & & & -1 \\ & & 1 & \end{pmatrix}; \quad J^{31} \equiv L^2 = \begin{pmatrix} 0 & & & \\ & & & 1 \\ & & 0 & \\ & -1 & & \end{pmatrix}; \quad J^{12} \equiv L^3 = \begin{pmatrix} 0 & & & \\ & & -1 & \\ & 1 & & \\ & & & 0 \end{pmatrix},$$

with the same commutation relations. Remark that

$$(L^1 + K^2)^2 = \begin{pmatrix} 1 & & & -1 \\ & 0 & & \\ & & 0 & \\ 1 & & & -1 \end{pmatrix} = (L^2 - K^1)^2$$

and $(L^1 + K^2)^3 = (L^2 - K^1)^3 = 0$.

It is advisable to pull these generators together in matrix form:

[8] Or by $K^a = -\frac{1}{2}\sigma^a$ and $L^a = -\frac{i}{2}\sigma^a$. In the usual terminology, $K^a = \frac{1}{2}\sigma^a$ and $K^a = -\frac{1}{2}\sigma^a$ correspond to the $D(0, \frac{1}{2})$ and $D(\frac{1}{2}, 0)$ spinor representations respectively, according to [19, Chap. 8].

$$J^{\mu\nu} = \begin{pmatrix} & K^1 & K^2 & K^3 \\ -K^1 & & L^3 & -L^2 \\ -K^2 & -L^3 & & L^1 \\ -K^3 & L^2 & -L^1 & \end{pmatrix} \quad \text{or} \quad J_{\mu\nu} = \begin{pmatrix} & -K^1 & -K^2 & -K^3 \\ K^1 & & L^3 & -L^2 \\ K^2 & -L^3 & & L^1 \\ K^3 & L^2 & -L^1 & \end{pmatrix}.$$

The general expression is $(J_{\rho\sigma})^{\alpha}_{\ \beta} = \delta^{\alpha}_{\rho}\, g_{\sigma\beta} - \delta^{\alpha}_{\sigma}\, g_{\rho\beta}$, and the commutation relations are summarized as:

$$[J_{\rho\sigma}, J_{\mu\nu}] = -g_{\rho\mu} J_{\sigma\nu} - g_{\sigma\nu} J_{\rho\mu} + g_{\sigma\mu} J_{\rho\nu} + g_{\rho\nu} J_{\sigma\mu}. \tag{12.16}$$

The dual tensor:

$$J^{*\rho\mu} := -\tfrac{1}{2}\varepsilon^{\rho\mu\nu\tau} J_{\nu\tau} = \begin{pmatrix} & -L^1 & -L^2 & -L^3 \\ L^1 & & K^3 & -K^2 \\ L^2 & -K^3 & & K^1 \\ L^3 & K^2 & -K^1 & \end{pmatrix}$$

plays a role in the theory of the WP. Notice that $\boldsymbol{K}\cdot\boldsymbol{L} = \frac{1}{2} J_{\rho\mu} J^{*\rho\mu}$ is a relativistic invariant; as is $\boldsymbol{K}^2 - \boldsymbol{L}^2 = \frac{1}{2} J_{\rho\mu} J^{\rho\mu} = -\frac{1}{2} J^{*}_{\rho\mu} J^{*\rho\mu}$. These are just the Casimirs of the Lorentz group. A generic infinitesimal Lorentz transformation is of the form

$$\Lambda \simeq 1 + \tfrac{1}{2}\omega^{\rho\sigma} J_{\rho\sigma}\,, \quad \text{or} \quad \Lambda^{\mu}_{\ \nu} = \delta^{\mu}_{\nu} + \omega^{\mu}_{\ \nu}\,,$$

where $\omega^{\rho\sigma}$ must be skewsymmetric.

The P^{μ} mutually commute. The remaining nonvanishing commutation relations for $\mathcal{P}$ are given by:

$$[L^a, P^b] = \varepsilon^{ab}_{\ \ c}\, P^c, \quad [K^a, P^b] = -\delta^{ab} P^0, \quad [K^a, P^0] = -P^a;$$

that is, $[J^{\kappa\rho}, P^{\mu}] = g^{\mu\rho} P^{\kappa} - g^{\mu\kappa} P^{\rho}$.

Let $U(\Lambda)$ be the unitary operator acting on one-particle states, corresponding to a Lorentz transformation Λ. As discussed for instance in [36, Sect. 2.4], one finds that

$$U^{\dagger}(\Lambda)\, \mathbb{P}^{\mu}\, U(\Lambda) = \Lambda^{\mu}_{\ \nu}\, \mathbb{P}^{\nu}; \quad U^{\dagger}(\Lambda)\, \mathbb{J}^{\mu\nu}\, U(\Lambda) = \Lambda^{\mu}_{\ \rho} \Lambda^{\nu}_{\ \sigma}\, \mathbb{J}^{\rho\sigma},$$

where by $\mathbb{P}$ and $\mathbb{J} = \{\mathbb{K}, \mathbb{L}\}$ we denote *hermitian* generators on Hilbert space, with commutation relations:

$$[\mathbb{L}^a, \mathbb{L}^b] = i\varepsilon^{ab}_{\ \ c}\, \mathbb{L}^c; \quad [\mathbb{L}^a, \mathbb{K}^b] = i\varepsilon^{ab}_{\ \ c}\, \mathbb{K}^c; \quad [\mathbb{K}^a, \mathbb{K}^b] = -i\varepsilon^{ab}_{\ \ c}\, \mathbb{L}^c;$$

that is, (12.16) leads to

$$[\mathbb{J}_{\rho\sigma}, \mathbb{J}_{\mu\nu}] = i\big(-g_{\rho\mu}\mathbb{J}_{\sigma\nu} - g_{\sigma\nu}\mathbb{J}_{\rho\mu} + g_{\sigma\mu}\mathbb{J}_{\rho\nu} + g_{\rho\nu}\mathbb{J}_{\sigma\mu}\big).$$

Appendix 2: The Lorentz Decompositions of Null Rotations

The unique decomposition of an arbitrary (proper orthochronous) Lorentz matrix S into the product of a rotation and a boost is well known [19, Chap. 1]. It becomes

$$\begin{aligned} S = \begin{pmatrix} \alpha & \boldsymbol{a}^t \\ \boldsymbol{c} & N \end{pmatrix} &= \begin{pmatrix} 1 & 0 \\ 0 & N - \boldsymbol{c}\boldsymbol{a}^t/(1+\alpha) \end{pmatrix} L_{\boldsymbol{a}/\alpha} \\ &=: \begin{pmatrix} 1 & 0 \\ 0 & N - \boldsymbol{c}\boldsymbol{a}^t/(1+\alpha) \end{pmatrix} \begin{pmatrix} \alpha & \boldsymbol{a}^t \\ \boldsymbol{a} & 1_3 + \frac{\boldsymbol{a}\boldsymbol{a}^t}{1+\alpha} \end{pmatrix}, \end{aligned}$$

where $\alpha^2 = 1 + \boldsymbol{a}^2$. Since S and S^t are Lorentz, which implies $N\boldsymbol{a} = \alpha\boldsymbol{c}$, $N^t\boldsymbol{c} = \alpha\boldsymbol{a}$ and $N^tN = 1_3 + \boldsymbol{a}\boldsymbol{a}^t$, one checks that $R := N - \boldsymbol{c}\boldsymbol{a}^t/(1+\alpha)$ is a rotation and that $R\boldsymbol{a} = \boldsymbol{c}$, and thus also $R + R\boldsymbol{a}\boldsymbol{a}^t/(1+\alpha) = N$.

We want to decompose null rotations in G_p. Note that there is an infinity of spacelike surfaces, of timelike, null or spacelike vectors, which are orbits of G_p in $\mathbb{M}$, each isometric to the group of motions of a plane [37]. Consider those null rotations which leave invariant the standard momentum $k = (1, 0, 0, 1)$. Denoting when convenient $b_1^2 + b_2^2$ by $|b|^2$, a general null rotation fixing k is given by:

$$S(b_1, b_2) := \begin{pmatrix} 1 + \frac{1}{2}|b|^2 & -b_2 & b_1 & -\frac{1}{2}|b|^2 \\ -b_2 & 1 & 0 & b_2 \\ b_1 & 0 & 1 & -b_1 \\ \frac{1}{2}|b|^2 & -b_2 & b_1 & 1 - \frac{1}{2}|b|^2 \end{pmatrix} =: \begin{pmatrix} \alpha & \boldsymbol{a}^t \\ \boldsymbol{c} & N \end{pmatrix}.$$

Simplifying further, we work out first the case $S(0, -b)$, with $b > 0$.

Here $\alpha^2 = 1 + b^2 + \frac{1}{4}b^4 = (1 + \frac{1}{2}b^2)^2$ so that $1 + \alpha = \frac{1}{2}(4 + b^2)$, and $S(0, -b)$ factorizes as

$$\begin{pmatrix} 1 + \frac{1}{2}b^2 & b & 0 & -\frac{1}{2}b^2 \\ b & 1 & 0 & -b \\ 0 & 0 & 1 & 0 \\ \frac{1}{2}b^2 & b & 0 & 1 - \frac{1}{2}b^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{4-b^2}{4+b^2} & 0 & -\frac{4b}{4+b^2} \\ 0 & 0 & 1 & 0 \\ 0 & \frac{4b}{4+b^2} & 0 & \frac{4-b^2}{4+b^2} \end{pmatrix} \begin{pmatrix} 1 + \frac{1}{2}b^2 & b & 0 & -\frac{1}{2}b^2 \\ b & 1 + \frac{2b^2}{4+b^2} & 0 & -\frac{b^3}{4+b^2} \\ 0 & 0 & 1 & 0 \\ -\frac{1}{2}b^2 & -\frac{b^3}{4+b^2} & 0 & 1 + \frac{b^4}{2(4+b^2)} \end{pmatrix}$$

$$=: RL = (RLR^{-1})R =: L'R.$$

We see clearly that R is a rotation around the y-axis, of positive angle θ turning anticlockwise from the positive z-axis towards the positive x-axis, with $\theta = 2\arctan(b/2)$. The velocity associated with the boost L' is:

$$\boldsymbol{v} = \big(2b/(2 + b^2), 0, -b^2/(2 + b^2)\big);$$

therefore its rapidity parameter is given by $\zeta = \operatorname{arcsinh}\big(\frac{1}{2}b\sqrt{4 + b^2}\big)$; the direction of the boost forms an angle $\arctan(b/2)$ with the x-axis, tilted towards the negative

z-axis. For small angles, it is intuitive that the boost undoes the turn effected by the rotation. The result reproduces the one indicated without proof in [32].

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Chapter 13
Dimensional Deception for the Noncommutative Torus

Fedele Lizzi and Alexandr Pinzul

Abstract We study the dimensional aspect of the geometry of quantum spaces. Introducing a physically motivated notion of the scaling dimension, we study in detail the model based on a fuzzy torus. We show that for a natural choice of a deformed Laplace operator, this model demonstrates quite non-trivial behaviour: the scaling dimension flows from 2 in IR to 1 in UV. Unlike another model with the similar property, the so-called Horava-Lifshitz model, our construction does not have any preferred direction. The dimension flow is rather achieved by a rearrangement of the degrees of freedom. In this respect the number of dimensions is deceptive. Some physical consequences are discussed.

Physical spacetime appears to be four a four-dimensional. Four dimension manifolds have very interesting structures, as it can be seen perusing *Wikipedia* [31]. Here we are making a long distance/low energy statement, since it is well known the possibility that there may be more dimensions curled and visible only at higher energies. These Kaluza-Klein theories are usually a byproduct of string theory (see for example [28]). There are good reasons, however, for which physicists may wish that the number of dimension actually *decreases*: gravity.

Gravity in four dimensions is a nonrenormalizable theory, in the perturbative series the diagrams which contain exchange of gravitons diverge. In two-dimensions, on the other side, gravity is a renormalizable theory, in fact the Einstein-Hilbert action is a topological invariant. It would therefore be nice to have a space which is

F. Lizzi (✉)
INFN, Sezione di Napoli & Dipartimento di Fisica "E. Pancini",
Università di Napoli Federico II, Napoli, Italy
e-mail: fedele.lizzi@na.infn.it

Departament de Física Quàntica i Astrofísica and Institut de Cíencies del Cosmos (ICCUB),
Universitat de Barcelona, Barcelona, Spain

A. Pinzul
Universidade de Brasília Instituto de Física & International Center of Physics,
Brasilia, DF, Brazil
e-mail: apinzul@unb.br

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_13

four dimensional at low energies, but two dimensional at high energies. A relevant attempt in this direction has been made in [13], but in this case the price to pay is to break Lorentz invariance, by picking up a definite direction and identify it with time. In this contribution we will present a space (a torus) which has an higher number of dimensions in the ultraviolet, compared with the infrared. The fundamental isometries are preserved, and in particular there is no need to choose a particular direction. This is not yet a realistic model of spacetime, the space is compact and Euclidean, but it is rather a "proof of concept". Also, in the ultraviolet the space is highly nontrivial and noncommutative, while in the infrared the noncommutativity can be rendered as small as wished. Most of what is presented here appeared in [19].

We will work in the algebraic description of geometry (and its generalizations) based on spectral triples [7, 8]. One starts with a set of data: an involutive algebra with certain properties of the norm, i.e. a C^*-algebra, $\mathscr{A}$ represented as bounded operators on a Hilbert space, $\mathscr{H}$, and a (non-necessarily bounded) operator $\mathscr{D}$, which is a generalization of the Dirac operator, and we will usually call Dirac operator tout court. This formulation leads immediately to nontrivial generalizations when the algebra is noncommutative, leading to *Noncommutative Geometries.* Accordingly we will define the dimension of a space in a purely spectral way, a definition originally due to Weyl. We will then show how a proper matrix approximation of a two dimensional torus will have two different limits, one is the long distance one, in which it appears two dimensional, in the other it will be, metrically speaking, the sum of two circles, hence a one dimensional space. It is important to notice that these two circles are not the circles whose product (not sum) give the torus. This is a phenomenon due to noncommutativity, recalling the presence of different phases in field theory [10, 12, 20, 24]. We will call matrix approximations of space "fuzzy", when they preserve the fundamental symmetries.

13.1 Dimensions à la Weyl

Let me first of all give the definition of dimension which is most useful for our purposes. It is due to Weyl and is based on the growth of the eigenvalues of the Laplacian. Let $N_\Delta(\omega)$ be the number, counting multiplicities, of eigenvalues of the Laplacian Δ on a compact Riemannian manifold, less then ω. Then there is only one value of d such that the following expression is finite

$$\lim_{\omega\to\infty} \frac{N_\Delta(\omega)}{\omega^{\frac{\mathrm{d}}{2}}} = \frac{\mathrm{Vol}(\mathscr{M})}{(4\pi)^{\frac{\mathrm{d}}{2}}\Gamma(\frac{\mathrm{d}}{2}+1)} \tag{13.1}$$

where Vol is the volume of the space, since we have a Laplacian we can define in fact a metric. The right hand side of (13.1) can actually be used to calculate the volume, admittedly in a rather elaborate way! This formula is purely spectral, and it

generalizes without any change to the noncommutative case. Clearly if the algebra is a finite dimensional one (a matrix algebra), the number of dimension $d = 0$.

Let us now calculate the dimension of the various kind of tori we will need in the following, commutative or otherwise. Consider first a flat commutative 2d torus $\mathbb{T}^2 = \mathbb{S}^1 \times \mathbb{S}^1$ with possibly different radii r and R. In Fourier transform the algebra of functions on this torus, i.e. the algebra which would appear in the spectral triple, is generated by two commuting generators: $u = \exp \frac{2\pi\,\mathrm{i}\,x}{r}$ and $v = \exp \frac{2\pi\,\mathrm{i}\,y}{R}$

$$\forall a \in \mathscr{A} \equiv \mathscr{C}^\infty(\mathbb{T}^2)\,, \quad a := \sum_{(l,m)\in\mathbb{Z}^2} a(l,m)\, u^l v^m\,, \tag{13.2}$$

continuity is ensured by the fast (Schwarzian) decay of the coefficients.

The passage to a noncommutative torus is done keeping the above expression but deforming the commutativity of the generators

$$VU = \mathrm{e}^{2\pi\,\mathrm{i}\,\theta}\, UV \tag{13.3}$$

for some real parameter θ called the deformation parameter. In the limit of $\theta \to 0$ one recovers the usual torus. We will call the algebra of the noncommutative torus generated by U and V as $\mathbb{T}^2_\theta$. It is an infinite dimensional algebra for alla values of θ, both rational or irrational.

For a generic θ the algebra of the noncommutative cannot be realized by finite matrices, but for $\theta = p/q$ rational there is a $q \times q$ matrix representation of U and V, and hence of the whole algebra which becomes just $\mathrm{Mat}_q(\mathbb{C})$. In this case the relation (13.3) is satisfied by the clock and shift matrices:

$$\mathscr{C}_q := \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & \mathrm{e}^{2\pi\,\mathrm{i}\,\theta} & 0 & \cdots & 0 \\ 0 & 0 & \mathrm{e}^{2\,2\pi\,\mathrm{i}\,\theta} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \mathrm{e}^{(q-1)\,2\pi\,\mathrm{i}\,\theta} \end{pmatrix}, \quad \mathscr{S}_q := \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 1 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{13.4}$$

These matrices are unitary, traceless and satisfy the relations $(\mathscr{C}_q)^q = (\mathscr{S}_q)^q = \mathbb{1}_q$, hence they generate $\mathbb{M}_q(\mathbb{C})$. We will call this particular noncommutative geometry a *fuzzy torus*.

Both the commutative and noncommutative torus have two (outer) derivations defined as

$$\begin{cases} \partial_1 U = 2\pi\,\mathrm{i}\,U\,,\ \partial_1 V = 0 \\ \partial_2 U = 0\,,\ \partial_2 V = 2\pi\,\mathrm{i}\,V \end{cases} \Leftrightarrow \begin{cases} \partial_1 a = 2\pi\,\mathrm{i} \sum\limits_{(l,m)\in\mathbb{Z}^2} l\, a(l,m)\, U^l V^m \\ \partial_2 a = 2\pi\,\mathrm{i} \sum\limits_{(l,m)\in\mathbb{Z}^2} m\, a(l,m)\, U^l V^m \end{cases}. \tag{13.5}$$

It is easy to see that the spectrum of the Laplacian is proportional to the sum of the square of two integers

$$Spec(\triangle_{com}) \propto \left\{ \frac{n_1^2}{r^2} + \frac{n_2^2}{R^2} \ , \ n_1, n_2 \in \mathbb{Z} \right\} \ . \tag{13.6}$$

and hence the Weyl dimension of is two for both commutative and noncommutative tori. The fuzzy torus does not have outer derivations, in particular does not have the analog of these derivations, but being a finite algebra it will anyway have dimension zero, at least at high enough energy (see below).

We now generalize Weyl's concept of dimension to define al effective, or scaling concept of dimension. The necessity of this generalization comes form a physical reasoning. The spectral dimension is an *concept*, i.e. it has to do with arbitrarily large scales, as the spectrum of the Laplacian has the dimensions of an energy. In reality no experiment can probe all scales up to infinity. Physically quantities, moreover, depend on the scale via the renormalization group. This leads to the definition of *scaling*dimension:

$$d(\omega) := 2\frac{d \ln N_\Delta(\omega)}{d \ln \omega} \ . \tag{13.7}$$

This is the dimension seen in experiments that probe the physics only up to the scale ω. The scale is defined in terms of the spectrum of a relevant physical Laplacian, the operator controlling the dynamics. The difference between the UV-dimension and the scaling can be seen when applied to any matrix geometry, i.e. when the relevant operators have finite spectra. The counting function in this case goes to a constant when $\omega \to \infty$. Any matrix geometry has a UV-dimension equal to zero. At the same time, it seems very natural that, if the spectrum is truncated at very high energy, we will not be able to tell the smooth geometry from the matrix one. Hence in any accessible experiment we will see the matrix geometry as a smooth one with some defined dimension, possibly with some "quantum" corrections. This observation makes the concept of a scaling dimension to be a very natural one, and it can be used for various physical tasks, for example in [11, 26].

Let us study a simplified model for which the number of dimensions can be deceptive. Start with the torus with two different radii, with the spectrum is given by (13.6). Introduce now some sort of "1-d fuzzyness" via the operator Δ_c diagonal in the basis above, but with the spectrum truncated on the direction of V at the integer N.

$$\Delta_c U^{n_1} = n_1^2 U^{n_1} \ , \quad \Delta_c V^{n_2} = \begin{cases} n_2^2 V^{n_2} & |n_2| \leq N \\ 0 & |n_2| > N \end{cases} \tag{13.8}$$

Clearly Δ_c is not a differential operator, and it does not have compact resolvent. The number N implicitly defines a length and therefore an energy scale. While in the R direction the Fourier series does not truncate, and therefore variation of arbitrarily small length can be taken into account, in the r direction only harmonics of width r/N contribute:

$$Spec(\triangle_{nc}) = \left\{ \frac{1}{R^2} \left(\mu^2 n_1^2 + n_2^2 \right) \ , \ n_1, n_2 \in \mathbb{Z} \ , \ |n_2| \leq N \right\} \tag{13.9}$$

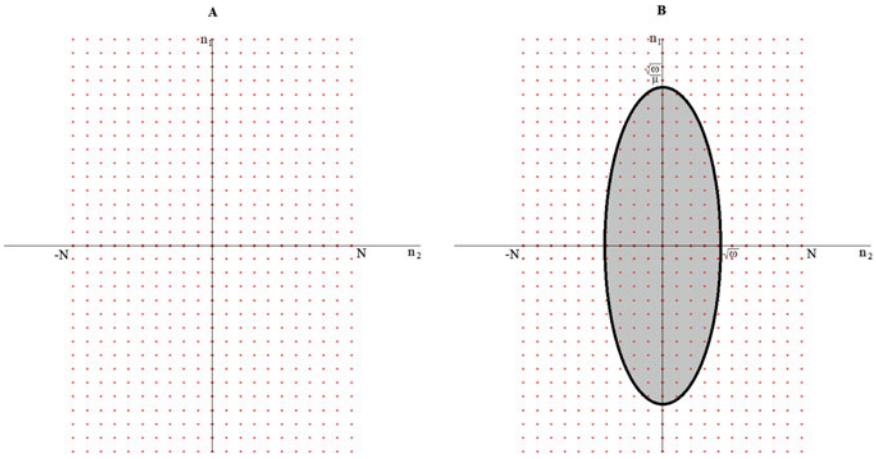

Fig. 13.1 **a** The structure of a typical spectrum with the n_2-direction truncated at N; **b** The solid curve $\mu^2 n_1^2 + n_2^2 = \omega$ represents a cut-off (we set $R = 1$). All the points of the spectrum inside the shadowed area are below the cut-off

The structure of a typical spectrum can be represented graphically as on Fig. 13.1a, while Fig. 13.1b gives the graphical answer for the counting function $N_\Delta(\omega)$: When $\mu \sim 1$ the low energy spectrum, up to N, is basically that of a two dimensional torus. The dimension is "deceptively" two, a low energy experiment will probe a two dimensional torus. When ω reaches N a transition phase starts.The number of dimensions decreases to one.

Consider now first the case $1 \ll \omega R^2 < \mu^2$ and at the same time $\omega R^2 < N^2$. The n_1 semi-axis of the cut-off ellipse is so small that no state with $n_1 \neq 0$ will contribute but the number of states with non-zero n_2 is enough to allow the application of the scaling dimension formula.

$$N_\Delta(\omega) \sim 2\sqrt{\omega}R \;\Rightarrow\; d(\omega) = 2\frac{d\ln N_\Delta(\omega)}{d\ln\omega} = 1 \tag{13.10}$$

We arrive at a very natural and expected result: if the experiment probes the scales below the energy needed to excite the first mode it does not see the corresponding compactified dimension.

Increasing the cut-off scale ω the states with $n_1 \neq 0$ will start contributing to the counting function. Only when a great number of them will enter, i.e. when $\omega R^2 \gg \mu^2$, (so one can pass from sum to integral) one can start using again the formula for scaling dimension to determine the dimension. This can happen either when

(a) ωR^2 is still less then N^2
(b) $\omega R^2 > N^2$ (but still of the order of N)
(c) $\omega R^2 \gg N^2$.

This is shown in Fig. 13.2.

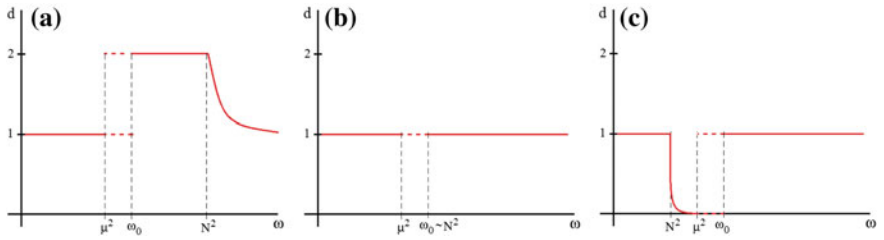

Fig. 13.2 The three cases for the spectrum of the operator (13.8) described in the text

We have seen that by changing the Laplacian it is possible to deceive the number of dimensions in a variety of ways. In all cases[1] however the dimension suppressed and the dimension where the original ones, and a choice has been made to suppress one of them. As in the case of Hořava-Lifshitz the fundamental symmetry of the space, which in this case is $U(1) \times U(1)$ acting as independent rotation on the two cycles, has been broken. We will now present a two dimensional model for which the number of dimensions is again going from two to one, but the high energy space retains the fundamental symmetry of space, and the single ultraviolet dimension emerges independently form the original two.

13.2 Matrix Approximations to the Noncommutative Torus

Our construction is based on approximating a torus by some sort of a *fuzzy* torus. Since these are nothing but matrix algebra one might think that the algebra of the noncommutative torus might be recovered as the inductive limit of $\mathrm{Mat}_q(\mathbb{C})$. This is however impossible, any indictive limit of finite algebra is approximatively finite, and there are mathematical results, based on K-theory, which show that this is impossible [30]. In [17, 25] it was clarified how one should construct and interpret the finite matrix approximation of the algebra of a noncommutative torus for an arbitrary θ. Because we will not use this construction in this work, we refer to [17] for all the details and to the reviews [21, 22] for the broader context.

There is however a construction, due to Elliott and Evans (EE) [9] which shows that the algebra of the noncommutative torus is the inductive limit of the algebra of two copies of the algebra of matrices whose entries are functions on a circle $\mathbb{T} \equiv \mathbb{S}^1$. Due to the presence of these functions, the algebra is not approximatively finite, and since the K-theory of a circle is $\mathbb{Z}$ there is the required matching of K-theories. Note

[1] There is one more case: $\mu \ll 1$. It can be analysed in the complete analogy with the ones we have considered. We will not describe it as it does not offer anything new.

however that at the finite level the algebra corresponds to a topological sum (not a product!) of two circles, i.e. a one-dimensional space.

Here we will just sketch the construction referring to the original paper [9] and to [19, Appendix] for details.

Consider a sequence of rational numbers converging to an irrational[2]:

$$\theta =: \lim_{n}\{\theta_n = p_n/q_n\} \tag{13.11}$$

then $q_n \to \infty$. The construction is based on the existence of a projection element of $P_{11} \in \mathbb{T}^2_\theta$, whose specific form and construction can be found in the original literature. What is important is the fact that it may be "translated" to build another element called P_{22}. The translation operation is simply a redifinition of the generators as $U \to \mathrm{e}^{p_n/q_n}\, U,\ V \to V$. This can be then iterated till $P_{q_nq_n}$. These elements will form the diagonal part of our matrix approximation. We then define the off diagonal elementsP_{21} as the unitary part of $P_{22}VP_{11}$, and so on for all P_{ij}.

By construction

$$P_{ij}P_{kl} = \delta_{jk}P_{il} \tag{13.12}$$

and it would seem that the P's might act as a basis for $\mathbb{M}(q_n, \mathbb{c})$, except that there is a fundamental caveat.

It is possible to obtain P_{1q_n} in two different ways: either as $P_{12}P_{23}\ldots P_{q_n-1\ q}$, or alternatively translating $q_n - 1$ times P_{21}. If these two operators were the same we would have constructed a subalgebra of $\mathbb{T}^2_\theta$ isomorphic to the matrix algebra $\mathrm{Mat}_q(\mathbb{C})$. They are not the same, but are related by a partial isometry z, so that the P_{ij}'s and z generate the algebra of matrix valued functions on the circle $\mathbb{M}_{q_{2n}}(\mathscr{C}^\infty(\mathbb{S}^1)) \subset \mathbb{T}^2_\theta$. Exchanging $U \leftrightarrow V$ (and after a unitary transformation) it is possible to obtain another set of matrix units and an isometry, orthogonal to the first one. The crucial point is that all these operators are element of the original algebra, and that as $n \to \infty$ we are just building a sequence of growing subalgebras.

To show[3] how the construction works let us define the following unitary elements of $\mathbb{T}^2_\theta$:

$$\mathrm{U}_n := \begin{pmatrix} \mathscr{C}_{q_{2n}} & 0 \\ 0 & \mathscr{S}_{q_{2n-1}}(z')^{-1} \end{pmatrix}, \quad \mathrm{V}_n := \begin{pmatrix} \mathscr{S}_{q_{2n}}(z) & 0 \\ 0 & \mathscr{C}_{q_{2n-1}} \end{pmatrix} \tag{13.13}$$

where $\mathscr{C}_q$ is an usual clock matrix, but$\mathscr{S}_q(z)$ is "almost" a shift matrix, where it not for the presence of the partial isometry z:

[2]The construction can be made, with little changes, also for theta rational.

[3]In the following, when there is no cause of confusion, we will sometime omit the subscript n from $q : n, q'_n$ and the like. This will render some formulas more explicit.

$$\mathscr{C}_q := \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & \omega_q & 0 & \cdots & 0 \\ 0 & 0 & \omega_q^2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \omega_q^{q-1} \end{pmatrix}, \quad \mathscr{S}_q(z) := \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 1 \\ z & 0 & 0 & 0 & 0 \end{pmatrix} \tag{13.14}$$

The two operators U_n and V_n generate the matrix algebra $\mathscr{A}_n$, which is nothing but two copies of the algebra of matrices of functions valued on a circle. The isometry z playing the role of $\mathrm{e}^{\mathrm{i}\varphi}$ generator:

$$\mathscr{A}_n \cong \mathbb{M}_{q_{2n}}(\mathscr{C}^\infty(\mathbb{S}^1)) \oplus \mathbb{M}_{q_{2n-1}}(\mathscr{C}^\infty(\mathbb{S}^1)) \tag{13.15}$$

The two operators satisfy a relation similar to the one of the original noncommutative torus. It is in fact an approximation of to which it converges to it in the limit $n \to \infty$.

$$\mathrm{V}_n\mathrm{U}_n = \omega_n \mathrm{U}_n\mathrm{V}_n\,, \quad \text{where } \omega_n = \begin{pmatrix} \omega_{q_{2n}}\mathbb{1}_{q_{2n}} & 0 \\ 0 & \omega_{q_{2n-1}}\mathbb{1}_{q_{2n-1}} \end{pmatrix} \tag{13.16}$$

The central point of the approximation is the fact that U_n and V_n converge *in norm* to the original U and V.

$$\lim_{n\to\infty} \|\mathrm{U}_n - U\| = \lim_{n\to\infty} \|\mathrm{V}_n - V\| = 0 \tag{13.17}$$

This enables the proof that the inductive limit of the algebras $\mathscr{A}_n$ is indeed the noncommutative torus

$$\lim_n \mathscr{A}_n = \mathbb{T}^2_\theta \tag{13.18}$$

The formal proof can be found in the original paper [9] or, with the notation used here, in [19]. Intuitively what happens is that the matrices U_n and V_n grow in size till filling up the whole og $\mathbb{T}^2_\theta$. The construction works also for the rational case (one can have a sequence of rational θ_n converging to another rational θ) [18, 29]. Note also that the algebras $\mathscr{A}_n$ are *not* approximatively finite, and that its K-theories are $\mathbb{Z} \oplus \mathbb{Z}$. It is therefore perfectly possible that they converge to the noncommutative torus, unlike a pure matrix algebra.

At a finite n the algebra $\mathscr{A}_n$ is the algebra of matrix valued the functions on two circles. Technically it is "Morita equivalent" to the algebra of complex valued functions on the two circles. Two Morita equivalent algebras have the same space of representations, with the same topology. At the same time it is possible to make the noncommutativity arbitrarily small. Such a space will be indistinguishable from two circles. In the next section we will also discuss the metric properties of this space.

The main characteristic of the construction is that *it preserves the symmetries of the original space.* While other constructions, (for example the Hořava-Lifshitz or Kaluza-Klein ones) in order to reduce the dimensions have to pick a preferred

direction (or directions), in our case the two circle are on an equal footing, and no direction has been chosem. The original fundamental symmetry of the torus of independently "rotate" the two cycles: $U \to \mathrm{e}^{i\alpha_1} U$, $V \to \mathrm{e}^{i\alpha_2} V$ is still a symmetry of the high energy space.

13.3 The Truncation Map

In this section we define a map (the truncation map) which associates to an element of the noncommutative torus an element of $\mathscr{A}_n$, i.e. a matrix valued function on two circles. In particular:

$$\forall a \in \mathscr{A}_\theta \ , \ \Gamma_n(a) := \sum_{(l,m)\in\mathbb{Z}^2} a(l,m)\, \mathrm{U}_n^l \mathrm{V}_n^m \tag{13.19}$$

since $(\mathscr{C}_q)^q = \mathbb{1}_q$, but $(\mathscr{S}_q(z))^q = z\mathbb{1}_q$. Defining $[\ldots]$ the integer part we have

$$\begin{aligned} a^{(n)}(m + \left[\frac{q}{2}\right], r; l) &:= \sum_{s\in\mathbb{Z}} a(sq+m, lq+r) \\ a'^{(n)}(m, r + \left[\frac{q}{2}\right]; s) &:= \sum_{l\in\mathbb{Z}} a(sq+m, lq+r) \end{aligned} \tag{13.20}$$

Rearranging the coefficients in order to explicitly see the functions on the circle we have:

$$\begin{aligned} \Gamma_n(a) :&= \left(\sum_{m,r=1}^{q_{2n}} \sum_{l\in\mathbb{Z}} a^{(n)}(m + \left[\frac{q_{2n}}{2}\right], r; l) z^l (\mathscr{C}_{q_{2n}})^m (\mathscr{S}_{q_{2n}}(z))^r \right) \\ &\oplus \left(\sum_{m',r'=1}^{q_{2n-1}} \sum_{l'\in\mathbb{Z}} a'^{(n)}(m', r' + \left[\frac{q_{2n-1}}{2}\right]; l') z'^{l'} (\mathscr{S}_{q_{2n-1}}(z'))^{m'} (\mathscr{C}_{q_{2n-1}})^{r'} \right) \\ &=: \mathbf{a}^{(n)}(z) \oplus \mathbf{a}'^{(n)}(z') \end{aligned} \tag{13.21}$$

where $\mathbf{a}$, $\mathbf{a}'$ are $q \times q$ matrices.

13.4 Derivations

The noncommutative torus has the two derivations defined in (13.5). The fuzzy torus, being a matrix algebra, it has plenty on inner derivations, just commutation with any element, but it does not have outer derivations, and in particular no derivation which could satisfy the equivalent of (13.5). However, it possible to define two *approximate*

derivations operators. We call call them approximate derivations because they close the Leibnitz rule on in the limit of large n.

It would be desirable that the derivations in $\mathscr{A}_n$ leave the P_n and P'_n invariant with their eigenspace, this means that the diagonal structure (13.13) is preserved under the derivation. One would like to have some consistent truncation or deformation of the standard derivations on $\mathscr{A}_\theta$ defined in (13.5).

Unfortunately it is impossible to define derivations of $\mathscr{A}_n$ with the same property and at the same time respecting the block-diagonal structure.[4] It is nevertheless possible to define two operators which well approximate the derivations. We call them ∇_i, $i = 1, 2$. The way to motivate (and find) is to consider a truncation of the usual derivations:

$$\nabla_i \Gamma_n(a) := \Gamma_n(\partial_i a) + \mathscr{O}(\cdots) \,, \tag{13.22}$$

where by $\mathscr{O}(\cdots)$ we denote the terms that vanish in the $q, q' \to \infty$ limit. The choice of these terms is made in such a way as to insure that the action of ∇_i is diagonal in the representation (13.21). Explicitly:

$$\begin{aligned}
\nabla_1 \Gamma_n(a) &:= 2\pi\, \mathrm{i} \left(\sum_{m,r=0}^{q_{2n}-1} \sum_{l\in\mathbb{Z}} \left(m - \left[\frac{q_{2n}}{2}\right] \right) a^{(n)}(m,r;l) z^l (\mathscr{C}_{q_{2n}})^{m-\left[\frac{q_{2n}}{2}\right]} (\mathscr{S}_{q_{2n}}(z))^r \right. \\
&\left. \oplus \sum_{m',r'=0}^{q_{2n-1}-1} \sum_{l'\in\mathbb{Z}} (l' q_{2n-1} + m')\, a'^{(n)}(m',r';l') z'^{l'} (\mathscr{S}_{q_{2n-1}}(z'))^{m'} (\bar{\mathscr{C}}_{q_{2n-1}})^{r'-\left[\frac{q_{2n-1}}{2}\right]} \right) \,, \\
\nabla_2 \Gamma_n(a) &:= 2\pi\, \mathrm{i} \left(\sum_{m,r=0}^{q_{2n}-1} \sum_{l\in\mathbb{Z}} (l q_{2n} + r)\; a^{(n)}(m,r;l) z^l (\mathscr{C}_{q_{2n}})^{m-\left[\frac{q_{2n}}{2}\right]} (\mathscr{S}_{q_{2n}}(z))^r \right. \\
&\left. \oplus \sum_{m',r'=0}^{q_{2n-1}-1} \sum_{l'\in\mathbb{Z}} \left(r' - \left[\frac{q_{2n-1}}{2}\right] \right) a'^{(n)}(m',r';l') z'^{l'} (\mathscr{S}_{q_{2n-1}}(z'))^{m'} (\bar{\mathscr{C}}_{q_{2n-1}})^{r'-\left[\frac{q_{2n-1}}{2}\right]} \right) .
\end{aligned} \tag{13.23}$$

The ∇_i are only *approximate* derivations because they satisfy the Leibnitz rule only in the limit of large n.

13.5 Weyl Dimension at Different Scales

We now ready to calculate the Weyl dimension of our space at different scales. Define first the deformed Laplacian $\Delta_{(n)}$ in the usual way as

[4] It is also true in the zero-dimensional approximation described in [17]. This is because (13.5) is incompatible with $(\mathscr{C}_q)^q = \mathbb{1}_q$.

$$\Delta_{(n)} = -\nabla_1^2 - \nabla_2^2 \,, \tag{13.24}$$

Since the general element of $\mathscr{A}_n$ can be written as $\Gamma_n(a)$ for some a, we have the eigenvalue problem:

$$-\left(\nabla_1^2 + \nabla_2^2\right)\Gamma_n(a) = \lambda\Gamma_n(a) \tag{13.25}$$

The eigenvalue problem can be rewritten as

$$\begin{aligned}
&\pi^2\left(\sum_{m,r=1}^{q_{2n}}\sum_{l\in\mathbb{Z}}\left(m^2+(q_{2n}l+r)^2\right)a^{(n)}(m+\left[\frac{q_{2n}}{2}\right],r;l)z^l(\mathscr{C}_{q_{2n}})^m(\mathscr{S}_{q_{2n}}(z))^r\right.\\
&\left.\oplus\sum_{m',r'=1}^{q_{2n-1}}\sum_{l'\in\mathbb{Z}}\left(r'^2+(q_{2n-1}l'+m')^2\right)a'^{(n)}(m',r'+\left[\frac{q_{2n-1}}{2}\right];l')z'^{l'}(\mathscr{S}_{q_{2n-1}}(z'))^{m'}(\mathscr{C}_{q_{2n-1}})^{r'}\right)\\
&=\lambda\left(\sum_{m,r=1}^{q_{2n}}\sum_{l\in\mathbb{Z}}a^{(n)}(m+\left[\frac{q_{2n}}{2}\right],r;l)z^l(\mathscr{C}_{q_{2n}})^m(\mathscr{S}_{q_{2n}}(z))^r\right.\\
&\left.\oplus\sum_{m',r'=1}^{q_{2n-1}}\sum_{l'\in\mathbb{Z}}a'^{(n)}(m',r'+\left[\frac{q_{2n-1}}{2}\right];l')z'^{l'}(\mathscr{S}_{q_{2n-1}}(z'))^{m'}(\mathscr{C}_{q_{2n-1}})^{r'}\right)
\end{aligned} \tag{13.26}$$

Using orthogonality relation among clock and shift

$$\mathrm{Tr}\left[(\mathscr{S}_q(z)^\dagger)^l(\mathscr{C}_q^\dagger)^p(\mathscr{C}_q)^m(\mathscr{S}_q(z))^r\right] = q\beta_q\delta_{lr}\delta_{pm} \,. \tag{13.27}$$

we can invert(13.26) to obtain, after some algebra,

$$\lambda = -4\pi^2\left(m^2+(q_{2n}l+r)^2\right) = 4\pi^2\left(r'^2+(q_{2n-1}l'+m')^2\right) \tag{13.28}$$

with

$$l,l'\in\mathbb{Z},\quad 1\le m,r\le q_{2n},\quad 1\le m',r'\le q_{2n-1} \tag{13.29}$$

This matching condition is a Diophantine relation. It is not sure that there are solution. In case of no solution it would mean that the spectrum is empty. Fortunately there are eigenvalues: Both, $(q_{2n-1}l'+m')$ and $(q_{2n}l+r)$, are bijective maps to $\mathbb{Z}$. For every value of l', r' there is only one choice of l, r such that $(q_{2n-1}l'+m') = (q_{2n}l+r)$. Since $q_{2n-1} < q_{2n}$ then $\forall r'\ \exists! r : r' = r$. This shows that the spectrum is

$$4\pi^2(m^2+s^2),\qquad 1\le m\le q_{2n-1},\quad s\in\mathbb{Z} \tag{13.30}$$

We are in the same situation of the simplified model described at the beginning, except that this time we did not artificially cut the spectrum of the Laplacian by hand, choosing a preferred direction. The spectrum can now easily be calculated in the two extreme limits, infrared and ultraviolet. What one should expect to see in this limits? The physical spectral dimension is the dimension as seen in the experiment that can probe the geometry up to some cut-off scale. The infrared limit should look as the

commutative geometry, i.e. we expect that the spectral dimension is this case should be 2.

In the ultraviolet limit, on the other side, we do not have, in general, enough intuition, used as we are to look at ordinary, commutative, geometry. In this case the actual calculation should provide us with some hints on where the fundamental, i.e. ultraviolet, degrees of freedom really live. We will see that this is the case.

IR Regime

The cut-off scale ω is below the characteristic quantum geometric scale. In the case of a toy model this scale was controlled by the number of the states along R-direction. In the present scale, this means that $\omega < q_{2n-1}^2$. Only the winding modes (from two circles) with $l, l' = -1, 0$ contribute. We immediately have for the counting function

$$N_\Delta(\omega) \sim \text{degeneracy} \times \int_{m^2+s^2 \leq \frac{\omega}{4\pi^2}} dm\, ds = \text{const} \times \omega \tag{13.31}$$

With our definition of scaling dimension we get

$$d_{IR} = 2 \tag{13.32}$$

This result is not unexpected, is the consequence of the fact that the *effective* radii of two circles are very small. Although we started with all the radii of the order of 1the contribution of (l, l')-mode to the spectrum is of the order of $q^2 \gg 1$ (where q is either q_{2n} or q_{2n-1}). This effectively reduces the radii of the"internal" circles by the factor of q.

UV Regime

In this case many of the $\mathbb{S}^1$ winding modes are excited, $l, l' \gg 1$. The hypothetical experiment can probe the physics up to the cut-off $\omega \gg q_{2n}^2$. In this case we have for the spectrum (in terms of l', m', r')

$$4\pi^2 \left(r'^2 + (q_{2n-1}l' + m')^2\right) = 4\pi^2 q_{2n-1}^2 l'^2 \left(1 + \mathcal{O}\left(\frac{1}{l'}\right)\right) \tag{13.33}$$

The counting function in this limit is

$$N_\Delta(\omega) \to \text{degeneracy} \times \int^{q_{2n-1}} dm\, dr \int_{-\frac{\sqrt{\omega}}{2\pi q_{2n-1}}}^{\frac{\sqrt{\omega}}{2\pi q_{2n-1}}} dk = \text{const} \times q_{2n-1}\sqrt{\omega} \tag{13.34}$$

We get the physical dimension in ultraviolet

$$d_{UV} = 1 \tag{13.35}$$

Consider now the factor q in the ultraviolet counting function $N \sim \sqrt{q^2_{2n-1}\omega}$. From the original Weyl theorem the effective size of the ultraviolet dimension is proportional to q, instead of being of order one or even of order of $1/q$. This "elongation" is due to the q^2 matrix degrees of freedom This is very suggestive: in the ultraviolet the new single dimension is fundamental and the two IR dimensions of the torus have disappeared. And we stress again that the single reduced dimension is not one of the original two.

13.6 Discussion and Conclusions

We have argued how a construction for the noncommutative torus can give a space which is effectively two dimensional at low scales, or large distances, while being at high scales, small distances, actually a two dimensional sum of tho circles. Although we have discussed a $2 \to 1$ reduction a $4 \to 2$ reduction is possible in a straightforward way, but its presentation would be looking quite messy. One can reduce $\mathbb{T}^4_\theta = \mathbb{T}^2_\theta \times \mathbb{T}^2_\theta$ to two two tori using a similar reduction, as well as a reducing a four torus to four circles.

There are other aspects, like the presence of fermions, which could unveil other interesting features, and in particular the role of the Dirac operator, as opposed to the Laplacian. In particular in noncommutative geometry the Dirac operator is fundamental for the construction of the spectral action [5, 6]. The spectral action approach was used in the Horava-Lifshitz context in [23, 27]. Another aspect is that the spectral can be obtained form the cancellation of anomalies [2–4, 14] or a ζ-function regularization [15]. The presence of spaces, such as the one described here, with a built-in cutoff, alter profoundly the field theory, and in particular the ultraviolet dynamics of bosons [1, 16]. The relations of this reduction with these deep ultraviolet studies in another promising issue.

Acknowledgements FL acknowledges the support of the COST action QSPACE, the INFN Iniziativa Specifica GeoSymQFT and Spanish MINECO under project MDM-2014-0369 of ICCUB (Unidad de Excelencia 'Maria de Maeztu').

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Chapter 14
Notions of Infinity in Quantum Physics

Fernando Lledó and Diego Martínez

Abstract In this article we will review some notions of infiniteness that appear in Hilbert space operators and operator algebras. These include proper infiniteness, Murray von Neumann's classification into type *I* and type *I I I* factors and the class of Følner C*-algebras that capture some aspects of amenability. We will also mention how these notions reappear in the description of certain mathematical aspects of quantum mechanics, quantum field theory and the theory of superselection sectors. We also show that the algebra of the canonical anti-commutation relations (CAR-algebra) is in the class of Følner C*-algebras.

Classifications 81T05 · 43A05 · 47L40

14.1 Introduction

In this article we will review some situations in which different notions of infinity manifest in quantum mechanics and quantum field theory. To begin let us recall some reasonable and basic definitions of finiteness in set theory (cf., [1, Introduction]). A set X can be called *finite* if any of these conditions holds:

Dedicated to Alberto Ibort on the occasion of his 60th birthday.

Supported by research projects MTM2017-84098-P and Severo Ochoa SEV-2015-0554 of the Spanish Ministry of Economy and Competition (MINECO), Spain.

F. Lledó (✉) · D. Martínez
Department of Mathematics, University Carlos III Madrid, Avda. de la Universidad 30, 28911 Leganés, Madrid, Spain
e-mail: flledo@math.uc3m.es

D. Martínez
e-mail: lumartin@math.uc3m.es

Instituto de Ciencias Matemáticas (ICMAT), C/ Nicolás Cabrera 13-15, 28049 Madrid, Spain

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_14

(**F1**) there is a bijection $\varphi\colon X \to \{1, \dots, n\}$ for some $n \in \mathbb{N}$;
(**F2**) there does not exist a (disjoint) partition $X = X_1 \sqcup X_2$ such that $|X| = |X_1| = |X_2|$, where $|\cdot|$ denotes the cardinality of a set;
(**F3**) every injective map $f\colon X \to X$ is surjective.

The characterization (**F1**) uses the external structure of the natural numbers and is constructive, while (**F2**) identifies finiteness through the absence of a certain kind of decomposition, which resembles a *paradoxical* decomposition. The last item (**F3**) refers to Dedekind's definition of finiteness and is intrinsic to the structure. All these ideas and, in particular, their negation, reappear in a very natural way in the context of linear operators and operator algebras. This is how they also enter in the description of some aspects of Quantum Theory.

For infinite sets on which, in addition, a dynamic is defined one can further classify the system according to the dichotomy *amenable* versus *paradoxical*. It must be highlighted that *dynamics* is here understood in a wide sense, such as the action of a group on a space or as the action of an algebra on itself by left multiplication. The idea of amenability was introduced in the context of group actions by von Neumann in 1929 (cf. [2]) and its absence in the action of the rotation group on the unit ball $B_1 \subset \mathbb{R}^3$ was recognized as a fundamental reason that explains the possibility of paradoxically decomposing B_1. This fact eventually came to be known as the *Banach-Tarski paradox* (cf., [3–5]). Since then this dichotomy amenable versus paradoxical has enriched many other fields including algebras, metric spaces and operator algebras. Roughly speaking, amenable structures have an internal approximation in terms of finite substructures (the so-called *Følner sequences*) that have controlled growth with respect to the dynamics considered. It is therefore clear that all finite structures are normally amenable, while infinite structures might be or not. We refer to [1, 6–12] for additional motivation and results on this body of work.

The aim of this article is to review some results showing the different *degrees of infiniteness* that appears in some situations in Quantum Theory. We also bring into this analysis the class of Følner C*-algebras that capture some aspects of amenability in the context of operator algebras. These algebras can be characterized in terms of a sequence of unital completely positive linear maps into matrices which are asymptotically multiplicative. We will show that the CAR-algebra is in this class. We begin reviewing some notions of infiniteness that appear in the description of Hilbert space operators and operator algebras. In particular we introduce notions of proper infiniteness and Murray von Neumann's classification into type *I* and type *III* factors. We also recall some important results in local quantum physics in relation to this topic, in particular, Borchers property or the construction of the field algebra in the theory of superselection sectors.

14.2 Operators and Operator Algebras in Hilbert Spaces

Let $\mathcal{H}$ be a complex separable Hilbert space and denote by $\mathcal{B}(\mathcal{H})$ the set of all bounded linear operators on $\mathcal{H}$. Given an operator $T \in \mathcal{B}(\mathcal{H})$, its *operator norm* is given by

$$\|T\| := \sup_{\|x\|=1} \|Tx\| , \tag{14.1}$$

where $\|x\|$ is the Hilbert space norm of the vector $x \in \mathcal{H}$ induced by the scalar product $\langle \cdot, \cdot \rangle$.

Example 1 (i) If $\mathcal{H} \cong \mathbb{C}^n$, then $\mathcal{B}(\mathcal{H}) \cong M_n(\mathbb{C})$. In this case, it is well known that any isometry is necessarily a unitary, i.e., for any $M \in \mathcal{B}(\mathcal{H})$ with $M^*M = \mathbb{1}$, then $MM^* = \mathbb{1}$. This realizes Dedekind's notion (**F3**) of finiteness in the context of linear maps, since any injective map must as well be surjective.

(ii) If $\mathcal{H} \cong \ell_2(\mathbb{N})$ (the Hilbert space of square summable sequences), denote its canonical basis by $\{e_i\}_{i\in\mathbb{N}}$. The infinite dimension of the Hilbert space has now several consequences that can be understood as a linear analogy to Hilbert's Hotel. The following examples of non-unitary isometries can be understood as a negation of the finiteness condition (**F3**) in the linear context.

(a) *Unilateral shift:* Let $Se_i := e_{i+1}, i \in \mathbb{N}$, i.e., $S \cong \begin{pmatrix} 0 & 0 & 0 & \dots \\ 1 & 0 & 0 & \dots \\ 0 & 1 & 0 & \dots \\ \vdots & \ddots & \ddots & \ddots \end{pmatrix}$. Then we have $S^*S = \mathbb{1}$, but $SS^* = \mathbb{1} - P_0$, where $P_0(\cdot) := \langle e_0, \cdot \rangle\, e_0$ is the range one projection onto the linear subspace $\mathbb{C} \cdot e_0$. In this case one says that $\mathbb{1}$ is an infinite projection (see Definition 1 below).

(b) *Generators of the Cuntz algebra:* define $S_1 e_i := e_{2i}$ and $S_2 e_i := e_{2i+1}$. These are isometries (i.e., $S_1^* S_1 = S_2^* S_2 = \mathbb{1}$) and satisfy, in addition,

$$S_1^* S_2 = 0 \quad \text{and} \quad S_1 S_1^* + S_2 S_2^* = \mathbb{1} .$$

In other words, the ranges of S_1 and S_2 are infinite dimensional and mutually orthogonal subspaces of $\ell^2(\mathbb{N})$, giving a negation of the finiteness condition (**F2**). In this case one says that $\mathbb{1}$ is a properly infinite projection (see Definition 1 below).

(iii) *Partial isometries:* A linear map $V : \mathcal{H} \to \mathcal{H}$ is a partial isometry if V^*V is an orthogonal projection, which is called *domain projection*. This condition directly implies that VV^* is also a projection, the so-called *range projection*. These partial isometries are a generalization of the notion of isometry.

Next we introduce two types of operator algebras that will be important for this article, namely, C*- and von Neumann algebras. General references on this topic are, e.g., [13] or [14, Chap. 2]. We call a *-subalgebra $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$ a *C*-algebra* if

it is closed with respect to the uniform topology, i.e., the topology defined by the operator norm $\|\cdot\|$ (cf., 14.1). Important examples of C*-algebras are those generated by isometries having mutually orthogonal ranges. For $n \geq 2$, the Cuntz algebra $\mathcal{O}_n$ (see [15]) is the essentially unique C*-algebra generated by isometries $S_1, \ldots, S_n$ satisfying

$$S_i^* S_j = \delta_{ij} \mathbb{1}, \quad i, j \in \mathbb{N}\,, \text{ and } \sum_{i=1}^{n} S_i S_i^* = \mathbb{1}\,.$$

Example 1 shows how these isometries can be realized as elements of $\mathcal{B}(\ell_2(\mathbb{N}))$.

A unital *-subalgebra $\mathcal{N} \subset \mathcal{B}(\mathcal{H})$ is a *von Neumann algebra* if it is closed under the weak operator topology. A useful and alternative way to understand this class of algebras is through the notion of commutant of a set of operators. If $\mathcal{S}$ is a self-adjoint subset of $\mathcal{B}(\mathcal{H})$ (i.e., if $S \in \mathcal{S} \subset \mathcal{B}(\mathcal{H})$, then $S^* \in \mathcal{S}$), then we denote by $\mathcal{S}'$ the *commutant* of $\mathcal{S}$ in $\mathcal{B}(\mathcal{H})$, i.e., the set of all operators in $\mathcal{B}(\mathcal{H})$ commuting with all elements in $\mathcal{S}$. Von Neumann's celebrated bicommutant theorem shows that a unital *-subalgebra $\mathcal{N} \subset \mathcal{B}(\mathcal{H})$ is a von Neumann algebra iff $\mathcal{N} = \mathcal{N}''$. Therefore, if $\mathcal{S}$ is a self-adjoint subset of $\mathcal{B}(\mathcal{H})$, then $\mathcal{S}''$ is the smallest von Neumann algebra containing $\mathcal{S}$. A von Neumann algebra $\mathcal{N}$ is called a *factor* if it has a trivial center, i.e., if $\mathcal{N} \cap \mathcal{N}' = \mathbb{C} \cdot \mathbb{1}$.

Any von Neumann algebra is generated as a norm-closed space by the set of its projections, which we denote by $\mathcal{P}(\mathcal{N})$. Therefore, the classification we are interested in of von Neumann algebras is based on the classification of $\mathcal{P}(\mathcal{N})$. For the purpose of this article, it is enough to assume that the von Neumann algebra $\mathcal{N}$ is a (nonzero) factor, since general von Neumann algebras can be canonically decomposed in terms of factors.

Definition 1 Let $\mathcal{N}$ be a factor and denote by $\mathcal{P}(\mathcal{N})$ its lattice of orthogonal projections in $\mathcal{N}$. All the following definitions are *modulo* $\mathcal{N}$, that is, depend on $\mathcal{N}$. For $P, Q \in \mathcal{P}(\mathcal{N})$ we say

(i) P is *minimal* if $P \neq 0$ and for any projection $P_0 \in \mathcal{P}(\mathcal{N})$, $P_0 \leq P$ implies either $P_0 = 0$ or $P_0 = P$.

(ii) $P \sim Q$ if there exists a partial isometry $V \in \mathcal{N}$ such that $P = V^*V$ and $Q = VV^*$. The relation $\sim$ is called also Murray von Neumann equivalence.

(iii) P is *finite* (mod $\mathcal{N}$) if the only projection $P_0 \in \mathcal{P}(\mathcal{N})$ with $P \sim P_0 \leq P$ is the projection P itself.
If P is not finite then it is called *infinite* (mod $\mathcal{N}$). That is, there is a $P_0 \in \mathcal{P}(\mathcal{N})$ such that $P \sim P_0 < P$, namely, P is equivalent to a proper subprojection of itself.
P is *properly infinite* if there exist $P_1, P_2 \in \mathcal{P}(\mathcal{N})$ such that $P \sim P_1 \sim P_2$, $P_1 + P_2 \leq P$ and $P_1 P_2 = 0$, i.e., $P_1\mathcal{H} \perp P_2\mathcal{H}$.

(iv) A factor $\mathcal{N}$ is called *finite* (respectively, *infinite* or *properly infinite*) if $\mathbb{1}$ is a finite (respectively, infinite or properly infinite) projection.

Remark 1 (a) The definition of finite, infinite and properly infinite projections can be stated similarly in the context of C*-algebras. It is clear from Example 1

that $\mathbb{1} \in M_n(\mathbb{C})$ is a finite projection. On the contrary $\mathcal{B}(\ell_2(\mathbb{N}))$ is an infinite C*-algebra via the equivalence $\mathbb{1} \sim \mathbb{1} - P_0 < \mathbb{1}$.
Finally, the Cuntz algebras $\mathcal{O}_n$ (and any C*-algebra containing them), are *the* prototypes of properly infinite C*-algebras, since we have from Example 1 that $S_1 S_1^* + \cdots + S_n S_n^* = \mathbb{1}$ while

$$\mathbb{1} = S_1^* S_1 = \cdots = S_n^* S_n \quad \text{and} \quad S_i^* S_j = \delta_{ij} \mathbb{1}.$$

(b) It follows from the definition that any minimal projection in a von Neumann algebra is automatically finite. The most prominent example of minimal projection is the range one projection $P_x(\cdot) := \langle x, \cdot \rangle x$, defined for any $x \in \mathcal{H}$ with $\|x\| = 1$.
It should be noted that if P is a minimal projection in a von Neumann algebra $\mathcal{N}$, then the corner algebra is one-dimensional, i.e., $P\mathcal{N}P = \mathbb{C}P$. Moreover, all minimal projections are equivalent.

According to the properties of the lattice of projections we mention next some large subclasses of factors.

Definition 2 Let $\mathcal{N}$ be a factor and $\mathcal{P}(\mathcal{N})$ its lattice of projections.

(i) $\mathcal{N}$ is said to be of *type I* if $\mathcal{P}(\mathcal{N})$ contains a minimal nonzero projection.
(ii) $\mathcal{N}$ is said to be of *type III* if $\mathcal{P}(\mathcal{N})$ contains no nonzero finite projection.

Type *III* factors show, roughly speaking, the highest degree of infiniteness. In fact, for this class of algebras any nonzero projection admits the following halving property (which can be understood as a negation of **F2** in the linear context).

Lemma 1 *Let $\mathcal{N}$ be a factor and $\mathcal{P}(\mathcal{N})$ its lattice of projections. Then $P \in \mathcal{P}(\mathcal{N})$ is infinite if and only if P admits the following decomposition*

$$P = (P - Q) + Q \quad \text{for some} \quad Q \leq P \quad \text{and} \quad P \sim Q \sim (P - Q)\,.$$

For simplicity we will focus in this article only on these two classes of factors. Type *II* factors (those having no minimal projections but having nonzero finite projections) are also important in describing certain aspects quantum theory (see, e.g., [16, 17]).

14.3 Følner C*-Algebras

Motivated by the dichotomy amenable versus paradoxical in group theory we will introduce in this section the class of Følner C*-algebras. These algebras correspond to the amenable groups, in the sense of having a good internal approximation in terms of matrices that have controlled growth with respect to the dynamics given by the

product. We will also define the notion of algebraic amenability and some relation to the class of Følner C*-algebras. These ideas will be used in the next section.

For the next definition, recall that a tracial state on a C*-algebra $\mathcal{A}$ is a positive and normalized functional $\tau\colon \mathcal{A} \to \mathbb{C}$ that satisfies the usual tracial property $\tau(AB) = \tau(BA)$ for any $A, B \in \mathcal{A}$. In the next definition we specify the subclass of amenable traces (see, e.g., [18, Chap. 6]).

Definition 3 Let $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$ be a unital and separable C*-algebra. $\mathcal{A}$ is called a *Følner C*-algebra* if it has an *amenable trace* τ, i.e., a tracial state on $\mathcal{A}$ that extends to a state ψ on $\mathcal{B}(\mathcal{H})$ that has $\mathcal{A}$ in its centralizer, i.e.,

$$\tau = \psi|_{\mathcal{A}} \quad \text{and} \quad \psi(XA) = \psi(AX)\ ,\ A \in \mathcal{A}\ ,\ X \in \mathcal{B}(\mathcal{H})\ .$$

From this definition it follows immediately that any unital C*-subalgebra of a Følner C*-algebra is again in this class and that any finite dimensional algebra is a Følner C*-algebra, since the usual normalized trace of a matrix will do.

Remark 2 The state ψ in the preceding definition is called *hypertrace* in the literature and this class of algebras is also referred as weakly hypertracial (see [19] and references therein). The preceding definition is equivalent to the intrinsic definition of an abstract Følner C*-algebra $\mathcal{A}$ in terms of a sequence of unital completely positive linear maps into matrices $\varphi_n\colon \mathcal{A} \to M_{k(n)}$ which are asymptotically multiplicative. This approach shows explicitly the finite approximation scheme of this class of algebras (cf., [20, Theorem 4.3]). Moreover, this class of algebras are also relevant in problems of spectral approximation (cf., [21–24]).

We will conclude by introducing the notion of algebraically amenable algebras. We will restrict to the case of subalgebras of C*-algebras, but the definition and results are true for arbitrary algebras over arbitrary fields (cf. [6, 11, 12]).

Definition 4 Let $\mathfrak{A} \subset \mathcal{A}$ be a *-subalgebra of a C*-algebra $\mathcal{A}$. We call $\mathfrak{A}$ algebraically amenable if there is a sequence $\{W_k\}_{k=1}^{\infty}$ of finite dimensional subspaces of $\mathfrak{A}$ satisfying

$$\lim_{k\to\infty} \frac{\dim(AW_k + W_k)}{\dim(W_k)} = 1\ ,\quad A \in \mathfrak{A}\ .$$

Next we mention an important relation between algebraic amenability and the class of Følner C*-algebras. For a complete proof we refer to [7, Theorem 3.17].

Theorem 1 *Let $\mathfrak{A} \subset \mathcal{A}$ be a dense *-subalgebra of a unital separable C*-algebra $\mathcal{A}$. If $\mathfrak{A}$ is algebraically amenable, then $\mathcal{A}$ is a Følner C*-algebra.*

14.4 Quantum Physics

In the mathematical description of a physical theory one needs to specify the set of observables, the set of states and, possibly, the family of symmetries of the theory,

typically described in terms of a group action. For a description of a quantum theory (as opposed to a classical theory) one can use the language of *non-commutative* operator algebras and their state space. Symmetries are then incorporated to this setting via a representation of the corresponding group in terms of automorphisms of the operator algebra. These representations are typically implemented in terms of unitary representations of the group (see, e.g., [14, Chaps. 2 and 3] or [25, Part I]). One of the conceptual advantages of (non-commutative) C*-algebras is the neat distinction between the abstract algebra, whose self-adjoint elements correspond to observables, and its state space and the corresponding representations on a concrete Hilbert space. This point of view particularly pays off in Quantum Field Theory, where there is an abundance of inequivalent representations associated with abstract observables (cf. [26]; see also Sect. 14.4.3 below).

14.4.1 Type I Algebras and Quantum Mechanics

The most elementary example of a type *I* factor is $\mathcal{B}(\mathcal{H})$, where $\mathcal{H}$ is a finite or (separable) infinite dimensional Hilbert space. Many situations in Quantum Mechanics can be described in terms of this example. Pure states correspond in this context to minimal projections and mixed states are described in terms of normalized and positive trace class operators.

We begin by making precise the fact that $\mathcal{B}(\mathcal{H})$ is, in fact, the prototype of this kind of factors. It is illustrative to give a sketch of the proof since it shows how the minimality condition is used.

Proposition 1 *Let $\mathcal{N} \subset \mathcal{B}(\mathcal{H})$ be a factor of type I. Then there exist separable Hilbert spaces $\mathcal{K}_1$ and $\mathcal{K}_2$ and a unitary $U : \mathcal{H} \to \mathcal{K}_1 \otimes \mathcal{K}_2$ with $U\mathcal{N}U^* = \mathcal{B}(\mathcal{K}_1) \otimes \mathbb{1}$.*

Proof Let $\{P_j\}_{j\in J} \subset \mathcal{P}(\mathcal{N})$ be a maximal family of mutually orthogonal minimal projections. By maximality it follows that $\mathcal{H} \cong \bigoplus_{j\in J} P_j\mathcal{H}$. Moreover, by minimality of projections, all P_i, P_j must be equivalent for any pair $i, j \in J$. Therefore, there are partial isometries $V_{1j} \in \mathcal{N}$ with $V_{1j}V_{1j}^* = P_1$ and $V_{1j}^*V_{1j} = P_j$, $j \in J$. This implies that $\mathcal{N}$ is generated by the set $\{V_{1j} \mid j \in J\}$ since we have

$$\mathcal{N} \ni N = \sum_{i,j\in J} P_i N P_j = \sum_{i,j\in J} \lambda_{ij} V_{1i}^* V_{1j} \ , \tag{14.2}$$

where the coefficients $\lambda_{ij} \in \mathbb{C}$ are specified by the relation

$$V_{1i} P_i N P_j V_{1j}^* \in P_1 N P_1 = \mathbb{C}P_1 \ , \tag{14.3}$$

which, again, uses the minimality of P_1. In fact, note that

$$V_{1i} P_i N P_j V_{1j}^* = \lambda_{ij} P_1 \quad \text{andhence} \quad P_i N P_j = \lambda_{ij} V_{1i}^* P_1 V_{1j}^* = \lambda_{ij} V_{1i}^* V_{1j} \ . \tag{14.4}$$

Finally, consider the discrete set $\mathcal{J} = \{1, 2, \ldots |J|\}$ with $|J| \in \mathbb{N} \cup \{\infty\}$ and define the unitary map

$$U^* \colon \ell_2(\mathcal{J}, P_1\mathcal{H}) \to \mathcal{H}$$

by means of $U^*\xi := \sum_j V_{1j}^* \xi_j$, where $\xi = (\xi_j)_{j=1}^{|J|} \in \ell_2(\mathcal{J}, P_1\mathcal{H})$. Using now the equivalence $\ell_2(\mathcal{J}, P_1\mathcal{H}) \cong \ell_2(\mathcal{J}) \otimes P_1\mathcal{H}$ one can show that the algebra generated by $\{UV_{1j}U^* \mid j \in J\}$ is isomorphic to $\mathcal{B}(\ell_2(\mathcal{J})) \otimes \mathbb{1}$, because

$$UV_{1i}^* U^* UV_{1j}U^* = UV_{1i}^* V_{1j} U^* \cong E_{ij} \otimes \mathbb{1}$$

where $\{E_{ij} \mid i, j \in J\}$ is a set of matrix units in $\ell_2(\mathcal{J})$.

Remark 3 From the results mentioned in Sect. 14.2 it is clear that $\mathcal{B}(\mathcal{H})$ with $\dim\mathcal{H} = \infty$ is an infinite as well as properly infinite C*-algebra. Nevertheless, observe that the structure of type I factors allows to have subalgebras of Følner type. For instance, take two non-commuting range one projections $P, Q \in \mathcal{B}(\mathcal{H})$, the von Neumann algebra generated by them will be finite-dimensional, and hence Følner. Note that this reasoning is not possible in the context type III von Neumann algebras.

14.4.2 The CAR-Algebra

In this section we give a proof that the C*-algebras associated to the canonical anti-commutation relations (CAR-algebras) are, in fact, Følner C*-algebras. We begin by recalling its definition and some standard properties (see, e.g., [14, Sect. 5.2.2]).

Let $\mathfrak{h}$ be a complex separable Hilbert space with scalar product $\langle \cdot, \cdot \rangle$. We denote by $\mathrm{CAR}(\mathfrak{h})$ the algebraically unique C*-algebra generated by $\mathbb{1}$ and $a(f)$, $f \in \mathfrak{h}$, such that the following relations hold:

(i) The map $\mathfrak{h} \ni f \mapsto a(f)$ is antilinear.
(ii) $a(f_1)a(f_2) + a(f_2)a(f_1) = 0\,,\ f_1, f_2 \in \mathfrak{h}\,.$
(iii) $a(f_1)a(f_2)^* + a(f_2)^* a(f_1) = \langle f_1, f_2 \rangle \mathbb{1}\,,\ f_1, f_2 \in \mathfrak{h}\,.$

The algebra $\mathrm{CAR}(\mathfrak{h})$ is simple, has a unique tracial state and satisfies $\|a(f)\| = \|f\|$ for any $f \in \mathfrak{h}$. In the proof of the next theorem we exploit the finite approximation structure of the CAR-algebra.

Proposition 2 *Let $\mathfrak{h}$ be a complex separable Hilbert space. Then $\mathrm{CAR}(\mathfrak{h})$ is a Følner C*-algebra and its unique tracial state is amenable.*

Proof If $\dim \mathfrak{h} = n < \infty$, then $\mathrm{CAR}(\mathfrak{h}) \cong M_{2^n}(\mathbb{C})$ and hence Følner because it is finite dimensional. If $\dim \mathfrak{h} = \infty$ we may describe the CAR-algebra as a uniformly hyper-finite algebra of type 2^∞ (see [13, III.5.4]). In fact, $\mathrm{CAR}(\mathfrak{h})$ is the inductive limit of finite-dimensional algebras $\mathcal{A}_n \cong M_{2^n}(\mathbb{C})$ with injective embedding

$$\mathfrak{A}_n \ni A \mapsto \begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix} \in \mathfrak{A}_{n+1}\,.$$

Consider the *-algebra $\mathfrak{A} := \cup_{n=1}^{\infty} \mathfrak{A}_n$, which is dense in CAR($\mathfrak{h}$). We will prove that $\mathfrak{A}$ is algebraically amenable (cf. Definition 4) and therefore, by Theorem 1, we conclude that CAR($\mathfrak{h}$) is a Følner C*-algebra. Define the finite dimensional subspaces (in fact subalgebras) $W_k := \mathfrak{A}_k$, $k \in \mathbb{N}$. Then, since any $A \in \mathfrak{A}$ is contained in $\mathfrak{A}_{k_0}$ for some $k_0 \in \mathbb{N}$ we conclude that for any $k \geq k_0$ we have $AW_k \subset W_k$, and therefore $\dim(AW_k + W_k) = \dim(W_k)$ and

$$\lim_{k\to\infty} \frac{\dim(AW_k + W_k)}{\dim(W_k)} = 1 \ .$$

Finally, since CAR($\mathfrak{h}$) has a unique tracial state it must be amenable.

14.4.3 Local Quantum Physics

In this subsection we address several manifestations of infinity that appear in quantum field theory. For this analysis we use the axiomatic approach proposed by Haag and Kastler in the sixties using the language of operator algebras (see, e.g., [27–30]), usually known as Algebraic Quantum Field Theory or Local Quantum Physics. In this formulation the observables become the primary objects of the theory and are described by selfadjoint elements in an abstract C*-algebra. Here one considers the observables to be localized in spacetime, which, in this article, we restrict to be the 4-dimensional Minkowski space. The fundamental object of study is a *net of von Neumann algebras* labeled by spacetime regions in $\mathbb{R}^4$. Concretely, we consider the *index set*

$$\mathcal{I} := \{\mathcal{O} \subset \mathbb{R}^4 \mid \mathcal{O} \ \text{ open and bounded region in Minkowski space}\}$$

and a *net of von Neumann algebras* is denoted by

$$\mathcal{I} \ni \mathcal{O} \mapsto \mathcal{N}(\mathcal{O}) \subset \mathcal{B}(\mathcal{H}) \ .$$

Associated with this net we can define the *global algebra* by $\mathcal{R} := \Big(\underset{\mathcal{O}\in\mathcal{I}}{\cup} \mathcal{N}(\mathcal{O}) \Big)''$.

We begin by recalling the axioms of the *vacuum representation*. The axioms specifying this representation of the net $\mathcal{I} \ni \mathcal{O} \mapsto \mathcal{N}(\mathcal{O})$ are physically motivated and have physical and mathematical consequences. These rules formalize general principles of relativistic quantum mechanics like, e.g., Poincaré covariance or causality. Characteristic for the vacuum state is its invariance under the Poincaré group and the (relativistic) spectrum condition.

(A1) *Isotony:* If $\mathcal{O}_1 \subset \mathcal{O}_2$ then $\mathcal{N}(\mathcal{O}_1) \subset \mathcal{N}(\mathcal{O}_2)$.
(A2) *Additivity:* If $\mathcal{O} = \cup_j \mathcal{O}_i$ then $\mathcal{N}(\mathcal{O}) = \Big(\cup_j \mathcal{N}(\mathcal{O}_j) \Big)''$.

(A2′) *Weak additivity:* For each $\mathcal{O}_0 \in \mathcal{K}$ we have $\Big(\bigcup_{a\in\mathbb{R}^4} \mathcal{N}(a+\mathcal{O}_0)\Big)'' = \mathcal{R}$.

(A3) *Causality:* If $\mathcal{O}_1 \perp \mathcal{O}_2$ (i.e., $\mathcal{O}_1$ and $\mathcal{O}_2$ are causally disjoint), then $\mathcal{N}(\mathcal{O}_1) \subset \mathcal{N}(\mathcal{O}_2)'$.

(A4) *Covariance:* There is a strongly continuous unitary representation of the universal cover of the proper orthocronous Poincaré group $\mathcal{G} := \mathbb{R}^4 \rtimes \mathrm{SL}(2,\mathbb{C})$, $U : \mathcal{G} \to \mathcal{U}(\mathcal{H})$ such that

$$\mathcal{N}(g\mathcal{O}) = \alpha_g(\mathcal{N}(\mathcal{O})) = U(g)\mathcal{N}(\mathcal{O})U(g)^{-1}\ , \quad \alpha_g \in \mathrm{Aut}\,\mathcal{R}\ ,\ g \in \mathcal{G}\ .$$

(A5) *Spectrum condition:* The spectrum of the generators of the space-time translations is contained in the closed forward light cone, i.e.,

$$\sigma\Big(U(\mathbb{R}^4)\Big) \subset V_+\ .$$

(A6) *Existence of a vacuum vector:* There exists a unit vector $\Omega \in \mathcal{H}$ (called the vacuum vector) such that

$$\Big(\cup_{\mathcal{O}\in\mathcal{K}}\mathcal{N}(\mathcal{O})\Big)\Omega \ \text{ is dense in } \mathcal{H} \quad \text{and} \quad U(g)\Omega = \Omega\ , g \in \mathcal{G}\ .$$

For concrete examples of nets satisfying these axioms we refer to the free-net construction in [31, 32] as well as references therein. An immediate and surprising consequence of this set of axioms is the so-called *Reeh-Schlieder Theorem*.

Theorem 2 *Let $\mathcal{I} \ni \mathcal{O} \mapsto \mathcal{N}(\mathcal{O}) \subset \mathcal{B}(\mathcal{H})$ be a net satisfying the axioms of the vacuum representation. For every nonempty region $\mathcal{O} \in \mathcal{I}$ the vacuum vector Ω is cyclic and separating for $\mathcal{N}(\mathcal{O})$, i.e., the set $\mathcal{N}(\mathcal{O})\Omega \subset \mathcal{H}$ is dense in $\mathcal{H}$ and, for any local operator $N \in \mathcal{N}(\mathcal{O})$, one has that $N\Omega = 0$ implies $N = 0$.*

This result implies, in particular, that any nonzero local projection in $\mathcal{N}(\mathcal{O})$ has (for any nonempty $\mathcal{O} \in \mathcal{I}$) a nonzero expectation value in the vacuum. Moreover, this result also shows that the vacuum in quantum field theory is entangled for any pair of local algebras $\mathcal{N}(\mathcal{O}_1), \mathcal{N}(\mathcal{O}_2)$ with $\mathcal{O}_1 \perp \mathcal{O}_2$. We refer, e.g., to [27, Sect. 1.3] for a complete proof of the Reeh-Schlieder theorem which makes explicit use of the covariance axiom, weak additivity and the spectrum condition. For additional motivation, results and references see [33, 34].

The next result is known as *Wightman's inequality*. Let $\mathcal{O}_1, \mathcal{O}_2 \in \mathcal{I}$ and denote by $\mathcal{O}_1 \Subset \mathcal{O}_2$ if $\mathcal{O}_1 \subset \mathcal{O}_2$ and the distance of $\mathcal{O}_1$ to the boundary of $\mathcal{O}_2$ is positive, i.e., $\mathrm{dist}(\mathcal{O}_1, \partial\mathcal{O}_2) > 0$.

Theorem 3 *Let $\mathcal{I} \ni \mathcal{O} \mapsto \mathcal{N}(\mathcal{O}) \subset \mathcal{B}(\mathcal{H})$ be a net satisfying the axioms of the vacuum representation and such that the global algebra $\mathcal{R}$ is non-Abelian. Then for any $\mathcal{O}_1 \Subset \mathcal{O}_2$ we have that $\mathcal{N}(\mathcal{O}_1) \subsetneq \mathcal{N}(\mathcal{O}_2)$.*

This result implies that for each $\mathcal{O} \in \mathcal{I}$ the local algebras $\mathcal{N}(\mathcal{O})$ are necessarily infinite dimensional, since for $\mathcal{O}_1 \Subset \mathcal{O}_2$ we must have $\dim_{\mathbb{C}}\mathcal{N}(\mathcal{O}_1) < \dim_{\mathbb{C}}\mathcal{N}(\mathcal{O}_2)$. A complete proof of Wightman's inequality can be found in [27, Sect. 1.4] which uses explicitly the isotony axiom as well as covariance and weak additivity.

Local algebras are not only infinite dimensional, they are typically type III (showing the highest degree of infiniteness). The change in relativistic quantum mechanics to a net of algebras localized in spacetime regions $\mathcal{O} \in \mathcal{I}$ forces the radical change to type III (as opposed to a type I description in quantum mechanics). For specific regions such as a space-like wedge or for theories which, in addition, have conformal covariance, it can be even shown that the local algebras correspond to the unique hyperfinite type III_1 factor (see, e.g., [28, Sect. V.6] for details).

We conclude this section mentioning Borchers property which implies that, generically, local algebras are almost type III. This property, which is strongly based on the positivity of the energy, is enough in many applications. For a proof we refer to [27, Sects. 1.11 and 1.12]. Before stating the next result, recall from Sect. 14.2 that for a von Neumann algebra is of type III all nonzero projections are equivalent to $\mathbb{1}$.

Theorem 4 *Let $\mathcal{I} \ni \mathcal{O} \mapsto \mathcal{N}(\mathcal{O}) \subset \mathcal{B}(\mathcal{H})$ be a net satisfying the axioms of the vacuum representation, with unique vacuum vector Ω. Assume $\mathcal{O}_1, \mathcal{O}_2 \in \mathcal{I}$ satisfy $\mathcal{O}_1 \Subset \mathcal{O}_2$ and that there exists an $\mathcal{O} \in \mathcal{J}$ with $\mathcal{O} \subset \mathcal{O}_1^{\perp} \cap \mathcal{O}_2$. Then for any nonzero projection $P \in \mathcal{N}(\mathcal{O}_1)$ we have*

$$P \sim \mathbb{1} \bmod \mathcal{N}(\mathcal{O}_2) \ .$$

As an application of type III structure appearing in quantum field theory we refer, e.g., to the explanation of Fermi's two atom system (cf. [35, 36]).

14.4.4 The Theory of Superselection Sectors

The theory of superselection sectors allows from an analysis of a physically motivated family of states to understand three central aspects in elementary particle physics: the composition of charges, the classification of particle statistics and the charge conjugation. In this final subsection we will mention briefly the role that Cuntz algebras play in this frame, confirming again the importance of properly infinite C*-algebras in quantum field theory. The theory of superselection sectors as stated by the Doplicher-Haag-Roberts (DHR) selection criterion [28, 37, 38], is formulated in the frame of local quantum physics and led to a profound body of work, culminating in the general Doplicher-Roberts (DR) duality theory for compact groups [39, 40].

The DHR criterion selects a distinguished class of "admissible" representations of a quasilocal algebra $\mathcal{A}$ of observables, which has trivial center $\mathcal{Z} := \mathcal{Z}(\mathcal{A}) = \mathbb{C}\mathbb{1}$. This class of representations specifies a so-called DR-category $\mathcal{T}$, which is a full subcategory of the category of endomorphisms of the C*-algebra $\mathcal{A}$. Furthermore,

from this endomorphism category $\mathcal{T}$ the DR-analysis constructs a C*-algebra $\mathcal{F} \supset \mathcal{A}$ together with a compact group action $\alpha\colon \mathcal{G} \ni g \to \alpha_g \in \mathrm{Aut}(\mathcal{F})$ such that:

- $\mathcal{A}$ is the fixed point algebra of this action;
- $\mathcal{T}$ coincides with the category of all "canonical endomorphisms" of $\mathcal{A}$, associated with the pair $\{\mathcal{F}, \alpha_{\mathcal{G}}\}$.

Physically, $\mathcal{F}$ is identified as a field algebra and $\mathcal{G}$ with a global gauge group of the system. The pair $\{\mathcal{F}, \alpha_{\mathcal{G}}\}$, which we call *Hilbert C*-system* (see below for a precise definition), is uniquely determined by $\mathcal{T}$ up to isomorphisms. Conversely, $\{\mathcal{F}, \alpha_{\mathcal{G}}\}$ determines uniquely its category of all canonical endomorphisms. Therefore $\{\mathcal{T}, \mathcal{A}\}$ can be seen as the abstract side of the representation category of a compact group, while $\{\mathcal{F}, \alpha_{\mathcal{G}}\}$ corresponds to the concrete side of the representation category of $\mathcal{G}$, and, roughly, any irreducible representations of $\mathcal{G}$ is explicitly realized within the Hilbert C*-system. One can state the equivalence of the "selection principle", given by $\mathcal{T}$ and the "symmetry principle", given by the compact group $\mathcal{G}$. This is one of the crucial theorems of the Doplicher-Roberts theory (see also [27, 30, 41] for additional results and motivation).

We conclude explaining the structure of Hilbert C*-systems. These are, roughly speaking, a very special type of C*-dynamical system $(\mathcal{F}, \alpha_{\mathcal{G}})$ that, in addition, contain the information of the representation category of the compact group $\mathcal{G}$. We denote the dual object of $\mathcal{G}$ by $\widehat{\mathcal{G}}$, which is defined as the set of (unitary) equivalence classes of continuous irreducible unitary representations of $\mathcal{G}$ (on complex separable Hilbert spaces). A Hilbert space $\mathcal{H} \subset \mathcal{F}$, where $\mathcal{F}$ is a unital C*-algebra, is called *algebraic* if the scalar product $\langle \cdot, \cdot \rangle$ of $\mathcal{H}$ is given by $\langle A, B \rangle \mathbb{1} := A^* B$ for $A,\ B \in \mathcal{H}$. Henceforth, we consider only finite-dimensional algebraic Hilbert spaces. The support of $\mathcal{H}$ is defined by $\mathrm{supp}\,\mathcal{H} := \sum_{j=1}^{d} \Psi_j \Psi_j^*$, where $\{\Psi_j \,\big|\, j = 1, \ldots, d\}$ is any orthonormal basis of $\mathcal{H}$. We consider here only algebraic Hilbert space $\mathcal{H}$ with $\mathrm{supp}\,\mathcal{H} = \mathbb{1}$. For any $D \in \widehat{\mathcal{G}}$ consider the following projection on $\mathcal{F}$

$$\Pi_D(\cdot) := \int_{\mathcal{G}} \chi_D(g) \alpha_g(\cdot)\, dg\ ,$$

where χ_D is the modified character of the class D, i.e., $\chi_D(g) := \dim(D)\ \mathrm{Tr}(D(g))$. The subspaces Π_D, $D \in \widehat{\mathcal{G}}$, are called spectral subspaces of $\mathcal{F}$. Note that if one chooses the trivial representation $\iota \in \widehat{\mathcal{G}}$, then the corresponding spectral subspace is the fixed point algebra

$$\Pi_\iota(\mathcal{F}) := \{A \in \mathcal{F} \mid \alpha_g(A) = A\ ,\ g \in \mathcal{G}\}\ ,$$

which in our context turns out to coincide with the C*-algebra $\mathcal{A}$.

Definition 5 A C*-dynamical $\{\mathcal{F}, \alpha_{\mathcal{G}}\}$ with a compact group $\mathcal{G}$ is called a **Hilbert C*-system** if for each $D \in \widehat{\mathcal{G}}$ there is an algebraic Hilbert space $\mathcal{H}_D \subset \Pi_D \mathcal{F}$, such that $\alpha_{\mathcal{G}}$ acts invariantly on $\mathcal{H}_D$, and the unitary representation $\alpha_{\mathcal{G}}|_{\mathcal{H}_D}$ is in the equivalence class $D \in \widehat{\mathcal{G}}$.

Note that any algebraic Hilbert space $\mathcal{H}_D$, $D \in \widehat{\mathcal{G}}$, generates a Cuntz algebra $\mathcal{O}_n$ with $n = \dim D$ which are all subalgebras of the field algebra $\mathcal{F}$. Moreover, any algebraic Hilbert space $\mathcal{H}_D$ specifies a canonical endomorphism of the fixed point algebra by

$$\rho_D(A) = \sum_{i=1}^{n} \Psi_i A \Psi_i^* \ ,$$

where $\{\Psi_i \,\big|\, i = 1, \ldots, n\}$ is any orthonormal basis of $\mathcal{H}_D$. Since the supp$\mathcal{H}_D = \mathbb{1}$ the canonical endomorphisms are also unital, i.e., $\rho_D(\mathbb{1}) = \mathbb{1}$.

Remark 4 In the DR-theory the center $\mathcal{Z}$ of the C*-algebra $\mathcal{A}$ plays a special role. If $\mathcal{A}$ corresponds to the inductive limit of a net of local C*-algebras indexed by open and bounded regions of Minkowski space, then the triviality of the center of $\mathcal{A}$ is a consequence of standard assumptions on the net of local C*-algebras. But, in general, the C*-algebra appearing in the DR-theorem does not need to be a quasilocal algebra and, in fact, one has to assume explicitly that $\mathcal{Z} = \mathbb{C}\mathbb{1}$ in this context (see [39, Theorem 6.1]). Therefore from a systematical point of view it is natural to study the properties and structural modifications of this rich theory if one assumes the presence of a nontrivial center $\mathcal{Z} \supset \mathbb{C}\mathbb{1}$. From a physical point of view one can interpret the elements of the center $\mathcal{Z}$ of $\mathcal{A}$ as classical observables contained in the quasilocal algebra. Nevertheless the effect of the presence of classical observables in superselection theory requires a more careful analysis of the corresponding fundamental axioms. We refer to [42–44] for an analysis of the DR-duality theory in the case the relative commutant of the corresponding Hilbert C*-system satisfies the following minimality condition:

$$\mathcal{A}' \cap \mathcal{F} = \mathcal{Z} \ .$$

Concrete realization of these systems in terms of Cuntz-Pimsner algebras, a class of properly infinite C*-algebras generalizing Cuntz algebras, can be found in [45].

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Chapter 15
Poisson-Nijenhuis Manifolds, Classical Yang-Baxter Equations, and Frobenius Algebras

F. Magri and T. Marsico

Abstract In this paper we describe in detail the class of linear Poisson-Nijenhuis manifolds. We prove that they are related to Drinfeld's bialgebras, classical Yang-Baxter equations, and noncommutative Frobenius algebras.

15.1 Introduction

Poisson-Nijenhuis manifolds are a particular class of bihamiltonian manifolds. They are characterized by the property of being endowed with two tensor fields $P\colon T^*M \to TM$ and $N\colon TM \to TM$, of type $(2,0)$ and $(1,1)$ respectively, which verify the following four conditions:

i. P is a Poisson bivector: this means that P is skew-symmetric, and that the value $P(dF, dG)$ of the bivector P on the differentials dF and dG of the functions F and G is a Poisson bracket.
ii. N is a Nijenhuis tensor: this means that the Nijenhuis's torsion of N vanishes.
iii. The product of N and P is a second bivector $Q = NP$.
iv. For any vector field X and any 1-form α the Poisson bivector P and the Nijenhuis tensor N verify the compatibility condition

$$[NX, P\alpha] - NLie_X(P)\alpha + P(Lie_X(N^*)\alpha - Lie_{NX}(\alpha)) = 0.$$

The third and fourth conditions entail that Q is a Poisson bivector. By the second condition this Poisson bivector is compatible with P. Therefore the manifold M is

Dedicated to Alberto Ibort on the occasion of his 60th birthday.

F. Magri (✉)
Dipartimento di Matematica ed Applicazioni, Università di Milano Bicocca, Milan, Italy
e-mail: franco.magri@unimib.it

T. Marsico
Liceo Classico Berchet, Milan, Italy

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_15

endowed with a pair of compatible Poisson bivectors, and hence is a bihamiltonian manifold. These claims have been proved in [5].

In this paper we investigate in detail the class of *linear* Poisson-Nijenhuis structures over a vector space V. We proceed in three steps:

i. In Sect. 15.2 we spell out the above four conditions in the linear setting characteristic of the present paper, and we prove that a vector space endowed with a linear Poisson-Nijenhuis structure is necessarily a Drinfeld's bialgebra. This means that both the vector space V and its dual V^* are Lie algebras, and that these Lie algebras are compatible in the sense of Drinfeld [2]. As is known, the concept of Drinfeld's bialgebra is a cornerstone of the theory of Lie-Poisson groups. Therefore one may consider this result as a geometrical introduction to Lie-Poisson groups from the viewpoint of bihamiltonian geometry.
ii. In Sect. 15.3 we assume that a certain cocycle in the Chevalley cohomology of the Lie algebra defined over V^* is a coboundary. In this way we introduce the subclass of *exact* linear Poisson-Nijenhuis manifolds. We show that the potential of the coboundary, which is a linear skew-symmetric map $E\colon V \to V^*$, verifies necessarily the classical modified Yang-Baxter equation or, in a more geometric language, that the Schouten bracket $[E, E]$ of this potential is ad-invariant with respect to the adjoint action of the Lie algebra of V^*. As is known, the classical Yang-Baxter equation has been used by Sklyanin and Semenov Tian Shansky to build the R-matrix approach to soliton equations [7, 8]. They have shown that the R-matrix is a basic tool to give soliton equations a Lax formulation. Thus, in the above result one may foresee a bridge between the Lax formulation and the bihamiltonian formulation of soliton equations.
iii. In Sect. 15.4, finally, the consequences of the vanishing of the torsion of N are systematically worked out. We prove that this condition obliges V^* to be an associative algebra. Under a mild additional assumption, we also show that V^* is, more precisely, a non-commutative Frobenius algebra.

By reverting the perspective, one may start from the algebraic standpoint of Frobenius algebras and construct a linear Poisson-Nijenhuis manifolds according to the following procedure.

Let V^* be a Frobenius algebra, that is a vector space endowed with a multiplication $x \cdot y$ and with a non-degenerate metric $g\colon V^* \times V^* \to \mathbb{R}$ satisfying the conditions:

i. The product is associative: $(x \cdot y) \cdot z = x \cdot (y \cdot z)$
ii. The metric is invariant with respect to the product: $g(x \cdot y, z) = g(x, y \cdot z)$

for all $x, y, z \in V^*$. We denote by $[x, y] = x \cdot y - y \cdot x$ the commutator associated with the multiplication $x \cdot y$, by ξ and η arbitrary elements of the dual space V, and by $ad^*_x \xi$ the coadjoint action of the Lie algebra $(V^*, [x, y])$ on its dual V. We denote as well by $S\colon V \to V^*$ the contravariant metric tensor associated with g. We assume to know a solution of the classical modified Yang-Baxter equation associated with the commutator $[x, y]$ and with the contravariant metric tensor S, that is a linear skew-symmetric maps $E\colon V \to V^*$ satisfying the equation

$$E(\mathrm{ad}^*_{E\xi}\eta - \mathrm{ad}^*_{E\eta}\xi) - [E\xi, E\eta] = [S\xi, S\eta]$$

for any choice of elements ξ and η in V. Furthermore, we denote by $\rho(x, y) = x \cdot y + y \cdot x$ the anti-commutator associated with the multiplication $x \cdot y$ on V^*, and by $\tau\colon V \times V \to V$ its pull-back from V^* to V through the metric g:

$$\rho(S\xi, S\eta) = S\tau(\xi, \eta) \qquad for \quad all \quad \xi, \eta \in V.$$

We use these multilinear maps to construct two tensor fields P and N on V. The Poisson bivector is defined by

$$P_v x = \mathrm{ad}^*_x v$$

The Nijenhuis tensor is defined by

$$N_v\xi = \mathrm{ad}^*_{E\xi} v + \tau(v, \xi),$$

where v, ξ, and x should be regarded as an arbitrary point, a constant vector field, and a constant 1-form on the manifold V.

Proposition 1 *The vector space V endowed with the above tensor fields is an exact linear Poisson-Nijenhuis manifold.*

This proposition will be proved in Sect. 15.4.

The purpose of the present paper is to convince the reader that the elaborate algebraic conditions gathered in the last Proposition are simply a specific form of the four geometric conditions listed at the beginning of this section, defining the class of Poisson-Nijenhuis manifolds. As a rule, when one assumes that the manifold is a vector space and the tensor fields depend linearly on the point of the manifold, the geometric conditions of the bihamiltonian theory (formulated in the geometric language of vector fields, 1-forms, commutators of vector fields and Lie derivatives) lose their standard appearance and become a set of algebraic conditions, very often having a Lie-theoretical meaning. It is this mechanism of conversion from geometry to algebra which allows to pass from the theory of Poisson-Nijenhuis manifolds to Drinfed's bialgebras, classical Yang-Baxter equations, and Frobenius algebras. This passage was already outlined in Chap. 4 of the Ph.D. thesis of Tiziana Marsico [6]. This paper is a new and up-to-date version of some results presented in that thesis.

15.2 Linear Poisson-Nijenhuis Manifolds

Let the manifold M be a vector space V. Let us denote by v a point of M, and by (ξ, η) and (x, y) arbitrary constant vector fields and constant 1-forms on M, that is elements of V and V^* respectively. Since the tangent space T_vM and the cotangent space T^*_vM at the point v of M are naturally identified with V and V^* respectively,

the Poisson bivector P: $T^*M \to TM$ and the Nijenhuis tensor field N: $TM \to TM$ are a pair of maps

$$P: M \times V^* \to V$$

$$N: M \times V \to V$$

which are linear in the second entry.

Definition 1 The Poisson-Nijenhuis structure is linear if the above maps are linear with respect to the first entry as well, that is if the corresponding tensor fields depend linearly on the point of the manifold.

Our aim is to work out the restrictions imposed to these bilinear maps by the four conditions defining a Poisson-Nijenhuis manifold. The answer is well-known in the case of a Poisson bivector. A classical result of the theory of Poisson manifolds tells us that the bivector P is a linear Poisson tensor if and only if V^* is a Lie algebra [4]. Let us denote by $[x, y]$ its commutator. Then

$$P_v = ad_x^* v. \tag{15.1}$$

A similar representation holds for the linear Nijenhuis tensor N. To make explicit this representation, it is suitable to split N into its symmetric and skew-symmetric parts by writing

$$N_v \xi = 1/2[v, \xi] + 1/2\sigma(v, \xi), \tag{15.2}$$

where σ: $V \times V \to V$ is a symmetric bilinear map with values in V. The reason to denote the skew-symmetric part of N by the symbol $1/2[v, \xi]$ is due to a well-known property of Nijenhuis tensor fields. It is known that each Nijenhuis tensor field defines a new Lie bracket (the deformed bracket)

$$[[X, Y]]_N = [[NX, Y]] + [[X, NY]] - N[[X, Y]]$$

on the algebra of vector fields on the manifold M. In the case of an affine manifold, the deformed bracket can be restricted to the subalgebra of constant vector fields , giving rise to a Lie bracket on V. Here, for clarity, we have used the symbol $[[X, Y]]$ to denote the commutator of vector fields on M (instead of the standard symbol $[X, Y]$) in order to distinguish the commutator $[[\xi, \eta]]$ of ξ and η, viewed as constant vector fields on M, from the commutator $[\xi, \eta]$ of ξ and η seen as elements of the Lie algebra V. A simple calculation based on the identities

$$[[\xi, \eta]] = 0$$

$$[[\xi, N_v \eta]] = N(\xi, \eta)$$

shows that the restriction of the deformed bracket on constant vector fields coincides with the skew-symmetric part of N:

$$[[\xi, \eta]]_N = [\xi, \eta]. \tag{15.3}$$

Therefore, if M is a linear Poisson-Nijenhuis manifold, both V and V^* are endowed with the structure of a Lie algebra: the commutators $[x, y]$ on V^* and $[\xi, \eta]$ on V coincide with the skew-symmetric parts of P and N respectively. The role of the symmetric part σ of N will be identified later on, in Sect. 15.4, by exploiting the following three Lemmas, each spelling out the implications of one of the conditions listed at the beginning of the paper, defining the class of Poisson-Nijenhuis manifolds.

Lemma 1 *The linear tensor field N on the vector space M has vanishing Nijenhuis's torsion if and only if its skew-symmetric part verifies the Jacobi's condition*

$$[[\xi, \eta], \theta] + [[\eta, \theta], \xi] + [[\theta, \xi], \eta] = 0 \tag{15.4}$$

and its symmetric part verifies the quadratic condition

$$\begin{aligned} &\Big(\sigma\big(\sigma(\xi, \eta), \theta\big) - \sigma\big(\sigma(\xi, \theta), \eta\big) - [\xi, [\eta, \theta]]\Big) \\ &+\Big(\sigma(\mathrm{ad}_\theta \xi, \eta) + \sigma(\xi, \mathrm{ad}_\theta \eta) - \mathrm{ad}_\theta \sigma(\xi, \eta)\Big) \\ &-\Big(\sigma(\mathrm{ad}_\eta \xi, \theta) + \sigma(\xi, \mathrm{ad}_\eta \theta) - \mathrm{ad}_\eta \sigma(\xi, \theta)\Big) = 0 \end{aligned} \tag{15.5}$$

Proof Recall that the vanishing of the torsion of N on a manifold M requires that the equation

$$[[NX, NY]] - N([[NX, Y]] + [[X, NY]]) - N[[X, Y]]) = 0$$

be satisfied for any pair of vector fields X and Y on M. On constant vector fields ξ and η

$$[[N_v \xi, N_v \eta]] = N(N(v, \xi), \eta) - N(N(v, \eta), \xi),$$

and therefore

$$\begin{aligned} [[N\xi, N\eta]] = &\frac{1}{4}[[v, \xi], \eta] + \frac{1}{4}[\sigma(v, \xi), \eta] + \frac{1}{4}\sigma([v, \xi], \eta) + \frac{1}{4}\sigma(\sigma(v, \xi), \eta) \\ &-\frac{1}{4}[[v, \eta], \xi] - \frac{1}{4}[\sigma(v, \eta), \xi] - \frac{1}{4}\sigma([v, \eta], \xi) - \frac{1}{4}\sigma(\sigma(v, \eta), \xi). \end{aligned}$$

Since

$$N_v[[\xi, \eta]]_N = \frac{1}{2}[v, [\xi, \eta]] + \frac{1}{2}\sigma(v, [\xi, \eta]).$$

one readily arrives to the condition

$$\begin{aligned}&\big([[v,\xi],\eta]+[[\eta,v],\xi]+[[\xi,\eta],v]\big)\\&\quad+\big(\mathrm{ad}_\xi\sigma(v,\eta)-\sigma(\mathrm{ad}_\xi v,\eta)-\sigma(v,[\xi,\eta])\\&\quad-\mathrm{ad}_\eta\sigma(v,\xi)+\sigma(\mathrm{ad}_\eta v,\xi)+\sigma(v,[\eta,\xi])+\\&\quad+\sigma(\sigma(v,\xi),\eta)-\sigma(\sigma(v,\eta),\xi)+[[\xi,\eta],v]\big)=0.\end{aligned}$$

To complete the proof, it is now enough to notice that the two brackets in this expression must vanish separately since they behave differently under the permutation of the arguments. The vanishing of the totally skew-symmetric part give the Jacobi's condition on $[\xi,\eta]$. The vanishing of the other bracket gives the condition on the symmetric part σ stated in the Lemma.

Lemma 2 *The linear tensor field N on the vector space M verifies the differential compatibility condition with the linear Poisson bivector P if and only if its skew-symmetric part verifies the condition*

$$[\mathrm{ad}^*_x\xi,\eta]_N+[\xi,\mathrm{ad}^*_x\eta]_N-\mathrm{ad}^*_x[\xi,\eta]_N=\mathrm{ad}^*_{\mathrm{ad}^*_\xi x}\eta-\mathrm{ad}^*_{\mathrm{ad}^*_\eta x}\xi \tag{15.6}$$

and its symmetric part verifies the condition

$$\mathrm{ad}^*_x\sigma(\xi,\eta)-\sigma(\mathrm{ad}^*_x\xi,\eta)-\sigma(\xi,\mathrm{ad}^*_x\eta)=\mathrm{ad}^*_{\mathrm{ad}^*_\xi x}\eta+\mathrm{ad}^*_{\mathrm{ad}^*_\eta x}\xi. \tag{15.7}$$

Proof Recall that the differential compatibility condition requires that the equation

$$[[NX,P\alpha]]-NLie_X(P)\alpha+P(Lie_X(N^*)\alpha-Lie_{NX}(\alpha))=0$$

be satisfied for any vector field X and any 1-form α on M, where the symbol Lie_X denotes the Lie derivative along X. To evaluate this expression, it is suitable to use the identity

$$\langle Y,Lie_X(N^*)\alpha-Lie_{NX}(\alpha)\rangle=\langle[[NX,Y]]+[[X,NY]]-N[[X,Y]],\alpha\rangle$$

where $\langle,\rangle$ is the pairing among vector fields and 1-forms on the manifold M. On a constant vector field ξ and a constant 1-forms x this identity gives

$$Lie_\xi(N^*)x-Lie_{N\xi}(x)=-\mathrm{ad}^*_\xi x \tag{15.8}$$

where the generator ad^*_ξ of the coadjoint action of V on V^* is defined, as usual, by the identity

$$\langle\mathrm{ad}^*_\xi x,\eta\rangle=-\langle x,\mathrm{ad}_\xi\eta\rangle=-\langle x,[\xi,\eta]\rangle.$$

Since

$$Lie_{\xi}(P)x = \mathrm{ad}^*_x\xi \tag{15.9}$$

and

$$2[[N\xi, Px]] = \mathrm{ad}^*_x([v,\xi] + \sigma(v,\xi)) - [\mathrm{ad}^*_x v, \xi] - \sigma(\mathrm{ad}^*_x v, \xi)$$

one may readily verify that the compatibility condition becomes

$$\begin{aligned}&\big([\mathrm{ad}^*_x v, \xi] + [v, \mathrm{ad}_x\xi] - \mathrm{ad}^*_x[v,\xi] + \mathrm{ad}^*_{\mathrm{ad}^*_\xi x} v - \mathrm{ad}^*_{\mathrm{ad}^*_v x}\xi\big) + \\ &+\big(\sigma(\mathrm{ad}^*_x v, \xi) + \sigma(v, \mathrm{ad}^*_x\xi) - \mathrm{ad}^*_x\sigma(v,\xi) + \mathrm{ad}^*_{\mathrm{ad}^*_\xi x} v + \mathrm{ad}^*_{\mathrm{ad}^*_v x}\xi\big) = 0.\end{aligned}$$

To complete the proof, it is now enough to notice that the two brackets in this expression must vanish separately, since the first bracket is skew-symmetric while the second bracket is symmetric in the permutation of the arguments v and ξ.

Lemma 3 *The algebraic compatibility condition $NP = PN^*$ is automatically verified in view of the previous compatibility condition. Hence it does not introduce any additional restrictions on N.*

Proof First notice the simple identity

$$2(NP)_v(x) = [v, \mathrm{ad}^*_x v] + \sigma(v, \mathrm{ad}^*_x v).$$

Thus, $NP = PN^*$ if and only if

$$\begin{aligned}&\langle y, [v, \mathrm{ad}^*_x v] + \sigma(v, \mathrm{ad}^*_x v)\rangle + \\ &+ \langle x, [v, \mathrm{ad}^*_y v] + \sigma(v, \mathrm{ad}^*_y v)\rangle = 0.\end{aligned}$$

But (15.7) entails that

$$2\langle y, \sigma(v, \mathrm{ad}^*_x v)\rangle = \langle [y,x], \sigma(v,v)\rangle - 2\langle y, \mathrm{ad}^*_{\mathrm{ad}^*_v x} v\rangle.$$

Thus the condition becomes:

$$\langle y, [v, \mathrm{ad}^*_x v] - \mathrm{ad}^*_{\mathrm{ad}^*_v x} v\rangle + \langle x, [v, \mathrm{ad}^*_y v] - \mathrm{ad}^*_{\mathrm{ad}^*_v y} v\rangle = 0.$$

Since

$$\langle y, [v, \mathrm{ad}^*_x v] - \mathrm{ad}^*_{\mathrm{ad}^*_v x} v\rangle = -\langle \mathrm{ad}^*_v y, \mathrm{ad}^*_x v\rangle + \langle \mathrm{ad}^*_v x, \mathrm{ad}^*_y v\rangle$$

one immediately realizes that the condition is automatically verified without any additional condition on N.

For further convenience, we collect all the informations obtained so far in the following Proposition.

Proposition 2 *A linear Poisson–Nijenhuis manifold is a pair of Lie algebras* $(V, [\xi, \eta])$ *and* $(V^*, [x, y])$ *together with a symmetric bilinear map* $\sigma\colon V \times V \to V$ *that satisfy the following three sets of conditions:*

On $[x, y]$*:*

$$1.\ [x, y] = -[y, x]$$
$$2.\ [[x, y], z] + [[y, z], x] + [[z, x], y] = 0$$

On $[\xi, \eta]$*:*

$$3.\ [\xi, \eta] = -[\eta, \xi]$$
$$4.\ [\xi, [\eta, \theta]] + [\eta, [\theta, \xi]] + [\theta, [\xi, \eta]] = 0$$
$$5.\ [\mathrm{ad}^*_x\xi, \eta] + [\xi, \mathrm{ad}^*_x\eta] - \mathrm{ad}^*_x[\xi, \eta] = \mathrm{ad}^*_{\mathrm{ad}^*_\xi x}\eta - \mathrm{ad}^*_{\mathrm{ad}^*_\eta x}\xi$$

On $\sigma(\xi, \eta)$*:*

$$6.\ \sigma(\xi, \eta) = \sigma(\eta, \xi)$$
$$7.\ \sigma(\sigma(\xi, \eta), \theta) - \sigma(\sigma(\xi, \theta), \eta) - [\xi, [\eta, \theta]] + (\sigma(\mathrm{ad}_\theta\xi, \eta) + \sigma(\xi, \mathrm{ad}_\theta\eta) - \mathrm{ad}_\theta\sigma(\xi, \eta)) + - (\sigma(\mathrm{ad}_\eta\xi, \theta) + \sigma(\xi, \mathrm{ad}_\eta\theta) - \mathrm{ad}_\eta\sigma(\xi, \theta)) = 0$$
$$8.\ -\sigma(\mathrm{ad}^*_x\xi, \eta) - \sigma(\xi, \mathrm{ad}^*_x\eta) + \mathrm{ad}^*_x\sigma(\xi, \eta) = \mathrm{ad}^*_{\mathrm{ad}^*_\eta x}\xi + \mathrm{ad}^*_{\mathrm{ad}^*_\xi x}\eta$$

The Poisson bivector P *is given by*

$$P_v x = \mathrm{ad}^*_x v$$

and the Nijenhuis tensor N *by*

$$N_v\xi = \frac{1}{2}[v, \xi] + \frac{1}{2}\sigma(v, \xi)$$

It may be noticed that the fifth condition means that the commutators $[\xi, \eta]$ on V and $[x, y]$ on V^* satisfy the compatibility condition defining a Drinfeld's bialgebra [3]. It remains thus proved that

Corollary 1 *A linear Poisson-Nijenhuis manifold is a Drinfeld's bialgebra.*

15.3 Classical Yang-Baxter Equations

An interesting consequence of the previous Corollary is the appearance of the classical Yang-Baxter equations within the theory of linear Poisson-Nijenhuis manifold. In this section we tersely review a few points of the theory of these equations to motivate the introduction of the subclass of *exact* linear Poisson-Nijenhuis manifolds. It is for this class of manifolds that we shall be able to establish a connection with Frobenius algebras in the following section.

Let us assume that the manifold M is the dual of a Lie algebra to account for the first two conditions listed above. In this way we fix the linear Poisson structure of our manifold. We concentrate on the problem of defining a commutator $[\xi, \eta]$ on V satisfying the next three conditions (3–4–5). We notice (following the theory of Drinfeld's bialgebras) that the fifth condition means that the map $\varepsilon\colon V^* \to V^* \wedge V^*$ defined by

$$\langle \xi, \varepsilon_x(\eta)\rangle = \langle x, [\xi, \eta]\rangle \tag{15.10}$$

is a cocycle in the Chevalley cohomology of the Lie algebra structure of V^*. The simplest case is when ε is a coboundary. This happens if there exists a linear skew-symmetric map $E\colon V \to V^*$ such that

$$[\xi, \eta] = \mathrm{ad}^*_{E\xi}\eta - \mathrm{ad}^*_{E\eta}\xi \tag{15.11}$$

We shall assume this relation as the definition of the the commutator $[\xi, \eta]$, and we say that the corresponding linear Poisson-Nijenhuis structure is *exact*. With this choice we satisfy the third and fifth conditions (for wathever choice of the potential E of the coboundary ε). It remains to check the fourth condition, that is the Jacobi's identity. To discuss this condition, it is convenient to introduce the 2-form on V with values in V^* defined by

$$[E, E](\xi, \eta) := E(\mathrm{ad}^*_{E\xi}\eta - \mathrm{ad}^*_{E\eta}\xi) - [E\xi, E\eta].$$

It is the algebraic form of the *Schouten bracket* of the bivector E with itself. It is then possible to show that the Jacobi's identity is equivalent to the ad-invariance of this bracket with respect to the adjoint action of the Lie algebra $(V^*, [x, y])$. Explicitly this means that the equation

$$\mathrm{ad}_x([E, E](\xi, \eta)) = [E, E](\mathrm{ad}^*_x\xi, \eta) + [E, E](\xi, \mathrm{ad}^*_x\eta) \tag{15.12}$$

holds true for every $x \in V^*$ and (ξ, η) in V. This condition is commonly referred to as the generalized (classical) Yang-Baxter equation.

To proceed, it is convenient to further restrict the class of manifolds considered, in order to simplify the form of th Yang-Baxter equation. We require that the Lie algebra $(V^*, [x, y])$, defining the Poisson bivector, be endowed with an ad-invariant metric. We denote by $S\colon V \to V^*$ the contravariant metric tensor, and we notice that S is

a symmetric linear invertible map from V to V^* which satisfies the ad*–invariance condition

$$\langle S\mathrm{ad}_x^*\xi, \eta\rangle + \langle S\xi, \mathrm{ad}_x^*\eta\rangle = 0. \tag{15.13}$$

A particular class of solutions of the generalized Yang-Baxter equation consists then of the linear skew-symmetric maps E: $V \to V^*$ for which

$$[E, E](\xi, \eta) = [S\xi, S\eta]. \tag{15.14}$$

This equation is known as the modified Yang-Baxter equation (the classical Yang-Baxter equation being simply the vanishing of the Schouten bracket). Owing to the ad^*-invariance of the contravariant metric tensor the modified equation implies the generalized one. The conclusion is that the solutions of the modified Yang-Baxter equation allow to construct a Lie algebra structure on the dual space V satisfying the third, fourth, and fifth conditions of the table written above. From a geometric standpoint this means that the solutions of the modified classical Yang-Baxter equation define the skew-symmetric part of the linear Nijenhuis tensor to be coupled to the Poisson bivector defined by $(V^*, [x, y])$. In this way we have solved half of our problem. It remains to characterize the symmetric part of N.

15.4 Frobenius Algebras

Before discussing the last three conditions (6–7–8) it is expedient to make a change of variables. In place of the symmetric bilinear map $\sigma(\xi, \eta)$, we introduce the new symmetric bilinear map

$$\tau(\xi, \eta) := \sigma(\xi, \eta) - (\mathrm{ad}_{E\xi}^*\eta + \mathrm{ad}_{E\eta}^*\xi)$$

which includes the potential E of the coboundary ε. The substitution of σ by τ allows to write the Nijenhuis tensor in the form

$$N_v\xi = \mathrm{ad}_{E\xi}^* v + \frac{1}{2}\tau(\xi, \eta). \tag{15.15}$$

At the same time it allows to simplify significantly the last two conditions (7–8). With a little bit of work it is, indeed, possible to reduce these conditions to the form

$$\mathrm{ad}_x^*\tau(\eta, \theta) = \tau(\mathrm{ad}_x^*\eta, \theta) + \tau(\eta, \mathrm{ad}_x^*\theta)$$

$$\tau(\tau(\xi, \eta), \theta) - \tau(\tau(\xi, \theta), \eta) = -\mathrm{ad}_{[E,E](\eta,\theta)}^*\xi$$

Let us consider first the second condition. Since E satisfies the modified Yang-Baxter equation it takes the form

$$\tau(\tau(\xi,\eta),\theta)-\tau(\tau(\xi,\theta),\eta)=-\mathrm{ad}^*_{[S\eta,S\theta]}\xi.$$

By means of the contravariant metric tensor S we can pull-back the bilinear map τ from V to V^*. Let us call ρ: $V^*\times V^*\to V^*$ the pull-back of τ

$$\rho(S\xi,S\eta)=S\tau(\xi,\eta).$$

Since the metric tensor is ad-invariant, the contravariant metric tensor verifies the condition

$$S\mathrm{ad}^*_y S^{-1}x+\mathrm{ad}_y x=0.$$

This property allows to eliminate the metric from the second condition. We are left with the remarkable equation

$$\rho(\rho(x,y),z)-\rho(\rho(x,z),y)=[[y,z],x] \tag{15.16}$$

Similarly the first condition can be reduced to the form

$$\mathrm{ad}_x\rho(y,z)=\rho(\mathrm{ad}_x y,z)+\rho(y,\mathrm{ad}_x z). \tag{15.17}$$

In this way we have transformed conditions (7–8) on the symmetric part σ of N, into a couple of conditions (15.16) and (15.17) pertaining to the Lie algebra $(V^*,[x,y])$. From the geometric standpoint this means that the compatibility conditions between P and N, characterizing the class of Poisson-Nijenhuis manifolds, impose a set of strong restrictions on the admissible linear Poisson bivectors. To complete our path towards Frobenius algebras, it only remains to work out the consequences of these restrictions. To this end, let us introduce on V^* the inner composition law

$$2x\cdot y=[x,y]+\rho(x,y). \tag{15.18}$$

It is easily checked that this composition law is *associative* on account of conditions (15.16) and (15.17):

$$(x\cdot y)\cdot z=x\cdot(y\cdot z). \tag{15.19}$$

Hence an exact linear Poisson-Nijenhuis structure is necessarily defined on an associative algebra.

Let us take this conclusion for granted, and let us try to reconstruct the whole linear Poisson-Nijenhuis structure starting from the datum of an associative algebra $(V,x\cdot y)$. For this, we have to run through all the previous steps in the reverse order. First, we set

$$[x,y]=x\cdot y-y\cdot x \tag{15.20}$$

$$\rho(x,y)=x\cdot y+y\cdot x. \tag{15.21}$$

The conditions (15.16) and (15.17) are automatically verified. Thus we have the general form of the bilinear map ρ. To reconstruct τ we need, furthermore , the ad^*- invariant contravariant metric S. For this reason, we require that the associative algebra be endowed with a metric which is invariant with respect to the multiplication in the algebra. In this way we fall over a Frobenius algebra. Finally, to reconstruct both the symmetric part σ and the skew-symmetric part $[\xi, \eta]$ of the Nijenhuis tensor field we need a solution of the modified Yang-Baxter equation. It remains thus proved that the problem of constructing an exact linear Poisson-Nijenhuis manifold on a vector space is equivalent to the problem of finding the solutions of the modified Yang-Baxter equation on a non-commutative Frobenius algebra, as claimed in Proposition 1. The proof of this Proposition is now complete.

15.5 Concluding Remarks

The paper has a rather limited and specific scope: to provide a geometric perspective for the theory of classical Yang-Baxter equation to be contrasted with the commonly accepted algebraic viewpoint. Accordingly many aspects of the theory have been left in the shadow. We want briefly mention three of them. The first concerns the presence of a spectral parameter in the Yang-Baxter equation [1, 8]. The role of this parameter is unclear from the geometric standpoint, where a specific pair of tensor fields is considered instead of a family depending on a parameter. One possibility to introduce the spectral parameter in the geometric approach is to look at linear Poisson-Nijenhuis manifolds defined on loop-algebras. In this way the spectral parameter would be naturally englobed into the theory as a constitutive element of the base manifold M. The suitability of a thorough study of this class of manifolds (from the geometric viewpoint) is the first point we want to stress. The second question concerns the existence of polynomial Poisson tensors of any order. Once a linear Poisson-Nijenhuis structure has been constructed on a vector space V, an infinite sequence of polynomial Poisson bivectors NP, N^2P, N^3P, and so on, appears naturally within the geometric approach. In the algebraic approach to the Yang-Baxter equations it is usual, instead, to consider two Poisson bivectors but no more: one linear and one quadratic. Where are the remaining Poisson bivectors in the algebraic approach? This is the second question we want to point out. Finally, the third question concerns the Lax formulation. It is a well known fact, inside the bihamiltonian approach to integrable systems, that the Nijenhuis tensor enjoys the same isospectral properties of a Lax matrix. Its spectrum remain invariant along the flow of the Hamiltonian dynamical systems that are naturally defined on a Poisson-Nijenhuis manifold according to the standard procedures of bihamiltonian geometry. This occurrence suggests a possible connection between the two concepts. Is it possible to foresee a relation between the Lax matrix and the matrix representing the Nijenhuis tensor field N in some specific basis? This question is completely open, as far as we know.

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Chapter 16
Hermite Polynomial Representation of Qubit States in Quantum Suprematism Picture

Margarita A. Man'ko and Vladimir I. Man'ko

Abstract We consider the Hermite polynomial representation (H-representation) of spin states for qubits and qudits in quantum suprematism picture, where the state geometry is illustrated by Triadas of Malevich's squares. We obtain an explicit connection of the density matrices of qubit states with the wave functions of two-dimensional harmonic oscillators and the probabilities identified with the states. We establish the connection of optical tomographic-probability distributions describing the oscillator states with qudit state tomograms.

16.1 Introduction

In quantum mechanics, the system pure states are identified with the state vectors [1] and the system mixed states, with density matrices or density operators [2, 3]. There are different representations for the state density operators. For qubits, the density matrices are usually parameterized by Bloch vectors, and the states are identified with points in the Bloch ball [4–6]. There exists the Jordan–Schwinger map [7, 8] of the matrix algebras, including the algebra of the $SU(2)$ group, onto the oscillator creation and annihilation operators. In view of this map for spin states which provide the basis for irreducible representation of the algebra of the $SU(2)$ group, one can describe all the states by the wave functions of two-mode oscillators. Such construction called the Hermite polynomial representation of spin states was proposed in [9]. Also recently the new quantum suprematism approach to qubit states was developed, where the states are identified with probabilities illustrated by Triadas of Malevich's squares on a plane [10–18].

M. A. Man'ko · V. I. Man'ko (✉)
Lebedev Physical Institute, Russian Academy of Sciences,
Leninskii Prospect 53, Moscow 119991, Russia
e-mail: manko@lebedev.ru; mankovi@lebedev.ru

M. A. Man'ko
e-mail: mmanko@lebedev.ru

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_16

In this approach, the matrix elements of density $N \times N$-matrices of qudit states are explicitly expressed in terms of the probabilities of artificial $(N^2 - 1)$ "classical" coins to have positions "UP" or "DOWN." Our aim in this paper is to demonstrate explicitly the connection of different representations of qudit states, including H-representation on the example of a qubit.

Also we employ the symplectic and optical tomographic probability representations [19] of oscillator's states, where the oscillator states are identified with fair probability distributions. In this context, we connect the quantum suprematism picture of qubit states with symplectic tomography of the oscillator states.

For qudit states, we obtain new entropic-information inequalities corresponding to the subadditivity and strong subadditivity conditions for bipartite and tripartite classical and quantum system states; see, for example, [20].

This paper is organized as follows.

In Sect. 16.2, we review the Jordan–Schwinger map. In Sect. 16.3, the spin states are given by oscillator wave functions, and in Sect. 16.4 we describe the H-representation of spin systems. We discuss the probabilities determining the qubit states in the quantum suprematism representation in Sect. 16.5 and study an explicit relation of the H-representation with the quantum suprematism approach in Sect. 16.6. Then, in Sect. 16.7, we develop the H-representation for qudits and derive new entropic inequalities and relations for Hermite polynomials. Finally, in Sect. 16.8 we present our conclusions and prospectives.

16.2 Jordan–Schwinger Map

In this section, we review the Jordan–Schwinger map of spin observables onto operator $\hat{\rho}$ acting in the Hilbert space of a two-mode harmonic oscillator. The creation $a_k^\dagger$ and annihilation a_k operators of the oscillator satisfy the commutation relations

$$\left[a_k, a_j^\dagger\right] = \delta_{kj}, \qquad \left[a_k, a_j\right] = 0, \qquad k, j = 1, 2. \tag{16.1}$$

Given three 2×2-matrices A_{jk}, B_{jk}, and C_{jk}, such that $[A, B] = C$. We construct three operators $\hat{A}$, $\hat{B}$, and $\hat{C}$, using the following explicit formulas:

$$\hat{A} = \sum_{j,k=1}^{2} (A)_{jk} \hat{a}_j^\dagger \hat{a}_k, \qquad \hat{B} = \sum_{j,k=1}^{2} (B)_{jk} \hat{a}_j^\dagger \hat{a}_k, \qquad \hat{C} = \sum_{j,k=1}^{2} (C)_{jk} \hat{a}_j^\dagger \hat{a}_k. \tag{16.2}$$

One can check that operators $\hat{A}$, $\hat{B}$, and $\hat{C}$ satisfy the commutation relation

$$\left[\hat{A}, \hat{B}\right] = \hat{C}. \tag{16.3}$$

Thus, we constructed the map of matrices A, B, and C onto operators $\hat{A}$, $\hat{B}$, and $\hat{C}$ acting in the Hilbert space of the oscillator states.

If the matrices A, B, and C are the spin-1/2 generators,

$$A = (\sigma_x + i\sigma_y)/2, \qquad B = (\sigma_x - i\sigma_y)/2, \qquad C = \sigma_z/2, \tag{16.4}$$

where σ_x, σ_y, and σ_z are Pauli matrices,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{16.5}$$

the operators $\hat{A}$, $\hat{B}$, and $\hat{C}$ read

$$\hat{A} = \hat{a}_1^\dagger \hat{a}_2, \qquad \hat{B} = \hat{a}_2^\dagger \hat{a}_1, \qquad \hat{C} = (\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2)/2. \tag{16.6}$$

In this case, their commutation relations provide known commutation relations of spin operators $\hat{S}_+ = \hat{a}_1^\dagger \hat{a}_2$ and $\hat{S}_- = \hat{a}_2^\dagger \hat{a}_1$, such that $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$ and $\hat{S}_z = \hat{C}$, where we assume the Planck constant $\hbar = 1$,

$$\left[\hat{S}_x, \hat{S}_y\right] = iS_z, \qquad \left[\hat{S}_y, \hat{S}_z\right] = iS_x, \qquad \left[\hat{S}_z, \hat{S}_x\right] = iS_y. \tag{16.7}$$

The Casimir operator $\widehat{\mathbf{S}}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2$ for the $SU(2)$ group takes the form

$$\widehat{\mathbf{S}}^2 = \frac{\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2}{2}\left(\frac{\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2}{2} + 1\right). \tag{16.8}$$

16.3 The Spin States in Terms of Oscillator's Wave Functions

The oscillator states $\mid n_1 n_2\rangle$, where $n_1, n_2 = 0, 1, 2, \ldots$, realize the basis of irreducible representation of the $SU(2)$ group for spin $s = (n_1 + n_2)/2, s = 0, 1/2, 1, \ldots$ For spin $s = 1/2$, the basis vectors $\mid 10\rangle$ and $\mid 01\rangle$ provide the oscillator wave functions

$$\psi_{1/2\ 1/2}(x_1, x_2) = \langle x_1 x_2 \mid 10\rangle = \sqrt{2/\pi}\, x_1 \exp\left[-(x_1^2 + x_2^2)/2\right], \tag{16.9}$$

$$\psi_{1/2\ -1/2}(x_1, x_2) = \langle x_1 x_2 \mid 01\rangle = \sqrt{2/\pi}\, x_2 \exp\left[-(x_1^2 + x_2^2)/2\right]. \tag{16.10}$$

For an arbitrary spin s, the wave functions $\psi_{sm}(x_1, x_2)$; $m = -s, -s+1, \ldots, s$, corresponding to the oscillator states, read

$$\psi_{sm}(x_1, x_2) = \frac{e^{-(x_1^2+x_2^2)/2}}{2^s\sqrt{\pi}} \cdot \frac{H_{s+m}(x_1)H_{s-m}(x_2)}{\sqrt{(s+m)!(s-m)!}}. \tag{16.11}$$

The parity of the state $\psi_{sm}(x_1, x_2)$ is $P = (-1)^{2s}$. The qubit states are odd states. Here, in (16.11), $H_{s+m}(x_1)$ and $H_{s-m}(x_2)$ are Hermite polynomials; they are determined by the generating function series expansion

$$e^{-t^2+2tx} = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(x). \tag{16.12}$$

For pure states, the density operators acting in the Hilbert space of the oscillator states $\hat{\rho}_{sm} =\mid sm\rangle\langle sm \mid$ have the following matrix form in the position representation:

$$\rho_{sm}(x_1, x_2, x_1', x_2') = \langle x_1, x_2 \mid \hat{\rho}_{sm} \mid x_1', x_2'\rangle$$
$$= \frac{\exp[-(x_1^2 + x_2^2 + x'^2_1 + x'^2_2)/2]}{4^s\pi\ (s+m)!(s-m)!} H_{s+m}(x_1)H_{s-m}(x_2)H_{s+m}(x_1')H_{s-m}(x_2'). \tag{16.13}$$

This matrix satisfies the normalization condition $\int \rho_{sm}(x_1, x_2, x_1, x_2)\ dx_1\ dx_2 = 1$, and the purity parameter $\widetilde{\mu}$ given by the integral

$$\widetilde{\mu} = \int \psi_{sm}(x_1, x_2, x_1', x_2')\psi_{sm}(x_1', x_2', x_1, x_2)\ dx_1\ dx_2\ dx_1'\ dx_2' \tag{16.14}$$

is equal to the unity, i.e., $\widetilde{\mu} = 1$.

16.4 *H*-Representation

In [9], the other representation for spin states was introduced using the standard star-product formalism with quantizer–dequantizer operators [21–25]. For a given density operator $\hat{\rho}^{(s)}$ with matrix elements $\rho^{(s)}_{mm'}$; $m, m' = -s, -s+1, \ldots, s-1, s$, where $s = 0, 1/2, \ldots$, we construct a symbol of the operator $w(x_1, x_2, \theta)$, using the dequantizer operator $\hat{U}(x_1, x_2, \theta)$; $0 \le \theta \le 2\pi$, namely,

$$w(x_1, x_2, \theta) = \mathrm{Tr}\left(\hat{\rho}^{(s)}\hat{U}^{(s)}(x_1, x_2, \theta)\right), \tag{16.15}$$

where the dequantizer operator reads

$$\hat{U}^{(s)}(x_1, x_2, \theta) =\mid x_1, x_2, \theta\rangle\langle x_1, x_2, \theta\ \mid, \tag{16.16}$$

and the vector $\mid x_1, x_2, \theta\rangle$ is given by the series

$$\mid x_1, x_2, \theta\rangle = \frac{e^{-(x_1^2+x_2^2)/2}}{2^s\sqrt{\pi}} \sum_{m=-1}^{s} e^{im\theta} \frac{H_{s+m}(x_1)H_{s-m}(x_2)}{\sqrt{(s-m)!(s+m)!}} \mid sm\rangle. \tag{16.17}$$

The density operator $\hat{\rho}^{(s)}$ is determined by symbols (16.15) through the quantizer operator $\hat{D}^{(s)}(x_1, x_2, \theta)$ as follows:

$$\hat{\rho}^{(s)} = \int_0^{2\pi} d\theta \int dx_1\, dx_2\, w(x_1, x_2, \theta)\, \hat{D}^{(s)}(x_1, x_2, \theta), \tag{16.18}$$

and the quantizer operator $\hat{D}^{(s)}(x_1, x_2, \theta)$ has the matrix elements

$$D^{(s)}_{mm'}(x_1, x_2, \theta) = \langle sm \mid \hat{D}^{(s)}(x_1, x_2, \theta) \mid sm'\rangle = \frac{e^{i(m-m')\,\theta}}{2^{2s+1}\pi}$$
$$\times \frac{\sqrt{(s+m)!(s+m')!(s-m)!(s-m')!}}{(2s+m+m')!(2s-m-m')!}\, H_{2s+m+m'}(x_1)\, H_{2s-m-m'}(x_2). \tag{16.19}$$

The quantizer operator $\hat{D}^{(s)}(x_1, x_2, \theta)$ satisfies the equality

$$\langle \hat{D}\rangle\langle \hat{D}\rangle = \langle \hat{D}\rangle, \tag{16.20}$$

where the mean value of the quantizer operator is determined by the symbol $w_\rho(x_1, x_2, \theta)$ of an arbitrary pure-state density operator $\hat{\rho}$ such that $\hat{\rho}^2 = \hat{\rho}$, i.e.,

$$\langle \hat{D}\rangle = \iint_0^{2\pi} \hat{D}^{(s)}(x_1, x_2, \theta) w_\rho(x_1, x_2, \theta)\, dx_1\, dx_2\, d\theta, \tag{16.21}$$

where $w_\rho(x_1, x_2, \theta)$ is the symbol of an arbitrary pure-state density operator $\hat{\rho}$.

16.5 Qubit State

We consider the example of qubit state with the density matrix

$$\rho = \begin{pmatrix} \rho_{1/2\ 1/2} & \rho_{1/2\ -1/2} \\ \rho_{-1/2\ 1/2} & \rho_{-1/2\ -1/2} \end{pmatrix}; \tag{16.22}$$

the density operator $\hat{\rho}$ of the state is represented by this matrix in the basis $\mid m\rangle$, where $m = \pm 1/2$ is the spin-1/2 projection on the z axis, i.e., $(\sigma_Z/2) \mid m\rangle = m \mid m\rangle$. This density matrix in the introduced H-representation with quantizer operator $\hat{D}$ in the basis (16.19) for spin $s = 1/2$ is expressed in terms of Hermite polynomials

$H_{1,2}(x)$ as follows:

$$\rho_{1/2\ 1/2} = \int_{-\infty}^{\infty}\int_{0}^{2\pi} w(x_1, x_2, \theta)\,\frac{H_2(x_1)}{8\pi}\,dx_1\,dx_2\,d\theta,$$
$$\rho_{1/2\ -1/2} = \int_{-\infty}^{\infty}\int_{0}^{2\pi} w(x_1, x_2, \theta)\,\frac{e^{i\theta}}{4\pi}\,H_1(x_1)\,H_1(x_2)\,dx_1\,dx_2\,d\theta,$$
$$\rho_{-1/2\ 1/2} = \int_{-\infty}^{\infty}\int_{0}^{2\pi} w(x_1, x_2, \theta)\,\frac{e^{-i\theta}}{4\pi}\,H_1(x_1)\,H_1(x_2)\,dx_1\,dx_2\,d\theta, \tag{16.23}$$
$$\rho_{-1/2\ -1/2} = \int_{-\infty}^{\infty}\int_{0}^{2\pi} w(x_1, x_2, \theta)\,\frac{H_2(x_2)}{8\pi}\,dx_1\,dx_2\,d\theta,$$

where the Hermite polynomials $H_1(z) = 2\,z$ and $H_2(z) = 4\,z^2 - 2$.

For the symbol of the density operator, we introduce the notation $w(x_1, x_2 \mid \theta) \equiv w(x_1, x_2, \theta)$. In the H-representation, the symbol of the density operator is determined by the matrix elements $\rho_{mm'}$ (16.22); it reads

$$w(x_1, x_2 \mid \theta) = \frac{e^{-(x_1^2+x_2^2)}}{2\pi}\Big[\rho_{1/2\ 1/2}\,H_1^2(x_1) + \rho_{-1/2\ -1/2}\,H_1^2(x_2) + \big(\rho_{1/2\ -1/2}\,e^{-i\theta} + \rho_{-1/2\ 1/2}\,e^{i\theta}\big)\,H_1(x_1)\,H_1(x_2)\Big]. \tag{16.24}$$

This function can be presented in the form

$$w(x_1, x_2 \mid \theta) = \frac{2e^{-(x_1^2+x_2^2)}}{\pi}\Big[\rho_{1/2\ 1/2}\,x_1^2 + \rho_{-1/2\ -1/2}\,x_2^2 + \big(\rho_{1/2\ -1/2}\,e^{-i\theta} + \rho_{-1/2\ 1/2}\,e^{i\theta}\big)\,x_1\,x_2\Big]. \tag{16.25}$$

The function is nonnegative $w(x_1, x_2 \mid \theta) \geq 0$ and normalized for an arbitrary phase θ, i.e., $\int_{-\infty}^{\infty} w(x_1, x_2 \mid \theta)\,dx_1\,dx_2 = 1$; it can be interpreted as the conditional probability density $w(x_1, x_2, \theta) \equiv w(x_1, x_2 \mid \theta)$, and we call it the H-tomogram of the qubit state (spin-1/2 state).

There exists the joint probability distribution of three random variables due to Bayes' formula [26]

$$W(x_1, x_2, \theta) = w(x_1, x_2 \mid \theta)\Pi(\theta), \tag{16.26}$$

where the probability density $1 \geq \Pi(\theta) \geq 0$ is an arbitrary nonnegative function such that $\int_0^{2\pi} \Pi(\theta)\,d\theta = 1$. We can choose this function as $\Pi(\theta) = (2\pi)^{-1}$.

In terms of the joint probability distribution $W(x_1, x_2, \theta)$, the density matrix is reconstructed, in view of the formula

$$\rho_{mm'}^{(s=1/2)} = \int_0^{2\pi} \int_{-\infty}^{\infty} \frac{W(x_1, x_2, \theta)\ D_{mm'}(x_1, x_2, \theta)}{\int W(x_1, x_2, \theta)\, dx_1\, dx_2}\, dx_1\, dx_2\, d\theta. \tag{16.27}$$

In the explicit form, we have

$$D_{1/2\ 1/2}(x_1, x_2, \theta) = \frac{2x_1^2}{\pi}\, e^{-(x_1^2+x_2^2)}, \quad D_{1/2\ -1/2}(x_1, x_2, \theta) = \frac{2x_1x_2}{\pi}\, e^{-(x_1^2+x_2^2-i\theta)},$$
$$D_{-1/2\ 1/2}(x_1, x_2, \theta) = \frac{2x_1x_2}{\pi}\, e^{-(x_1^2+x_2^2+i\theta)}, \quad D_{-1/2\ -1/2}(x_1, x_2, \theta) = \frac{2x_2^2}{\pi}\, e^{-(x_2^2+x_2^2)}. \tag{16.28}$$

Since $w(x_1, x_2 \mid \theta)$ is the conditional joint probability distribution of two random variables, there exist two marginal probability distributions

$$\mathscr{P}_1(x_1) = \int w(x_1, x_2 \mid \theta)\, dx_2, \quad \mathscr{P}_2(x_2) = \int w(x_1, x_2 \mid \theta)\, dx_1; \tag{16.29}$$

they read

$$\mathscr{P}_1(x_1) = \frac{2e^{-x_1^2}}{\sqrt{\pi}} \left[\rho_{1/2\ 1/2} x_1^2 + \rho_{-1/2\ -1/2}/2\right],$$
$$\mathscr{P}_2(x_2) = \frac{2e^{-x_2^2}}{\sqrt{\pi}} \left[\rho_{-1/2\ -1/2} x_2^2 + \rho_{1/2\ 1/2}/2\right]. \tag{16.30}$$

The dependence on the angle θ in the marginal distributions disappeared, since the off-diagonal elements in (16.25) give zero contributions into (16.30).

Also the joint probability distribution $W(x_1, x_2, \theta)$ (16.26) determines the marginal joint probability distribution of two random variables $W(x_1, x_2)$ as follows:

$$W(x_1, x_2) = \int_0^{2\pi} W(x_1, x_2, \theta)\, d\theta = \frac{2e^{-(x_1^2+x_2^2)}}{\pi} \left[\rho_{1/2\ 1/2}\, x_1^2 + \rho_{-1/2\ -1/2}\, x_2^2 \right.$$
$$\left. + \left(\rho_{1/2\ -1/2} + \rho_{-1/2\ 1/2}\right) \langle \cos\theta \rangle + i \left(\rho_{1/2\ -1/2} + \rho_{-1/2\ 1/2}\right) \langle \sin\theta \rangle \right], \tag{16.31}$$

where

$$\langle \cos\theta \rangle = \int_0^{2\pi} \Pi(\theta) \cos\theta\, d\theta, \qquad \langle \sin\theta \rangle = \int_0^{2\pi} \Pi(\theta) \sin\theta\, d\theta; \tag{16.32}$$

for $\Pi(\theta) = 1/(2\pi)$, $\langle \cos\theta \rangle = \langle \sin\theta \rangle = 0$.

16.6 Quantum Suprematism Representation of Qubit States

In [10–12, 15–18], the quantum suprematism representation of qubit states was investigated. This representation is based on the possibility to express the density matrix of spin-1/2 states $\rho = \begin{pmatrix} \rho_{1/2\ 1/2} & \rho_{1/2\ -1/2} \\ \rho_{-1/2\ 1/2} & \rho_{-1/2\ -1/2} \end{pmatrix}$ in terms of three probabilities of spin projections $m = +1/2$ onto the x, y, and z axes [27]. The density matrix reads [10]

$$\rho = \begin{pmatrix} p_3 & p_1 - (1/2) - i(p_2 - 1/2) \\ p_1 - (1/2) + ip_2 - 1 & 1 - p_3 \end{pmatrix}, \tag{16.33}$$

where $1 \geq p_1, p_2, p_3 \geq 0$ are the probabilities of spin projections $m = +1/2$ onto the x, y, and z axes, respectively. These probabilities satisfy the nonnegativity condition of the density matrices of the form

$$(p_1 - 1/2)^2 + (p_2 - 1/2)^2 + (p_3 - 1/2)^2 \leq 1/4; \tag{16.34}$$

for pure states, this inequality converts to the equality

$$(p_1 - 1/2)^2 + (p_2 - 1/2)^2 = p_3(1 - p_3). \tag{16.35}$$

The numbers p_1, p_2, and p_3 determine the three simplexes, which form the sides of equilateral triangle; the length of the triangle sides is equal to $\sqrt{2}$. On the sides of the triangle, there are three points $\mathscr{A}_1$, $\mathscr{A}_2$, and $\mathscr{A}_3$, which provide the vertices of another triangle; see Fig. 16.1.

There is the one-to-one correspondence of the density matrix (16.33) and the triangle $\mathscr{A}_1\mathscr{A}_2\mathscr{A}_3$ with the sides of the length

$$\ell_k = 2\left[1 + p_k^2 - 2\,p_k - p_{k+1} + p_{k+1}^2 + p_k p_{k+1}\right]; \quad k = 1, 2, 3; \quad p_4 \equiv p_1. \tag{16.36}$$

Three squares (black, red, and white) with areas $S_k = \ell_k^2$ correspond to the density matrix and they were called *Triada of Malevich's squares* [10–12, 17]; the sum of areas of the squares $S(p_1, p_2, p_3) = \ell_1^2 + \ell_2^2 + \ell_3^2$ has the maximum and minimum values; these values are $S_{\min} = 3/2$ and $S_{\max} = 3$ [17].

The minimum value corresponds to an equilateral triangle with vertices $\mathscr{A}_1$, $\mathscr{A}_2$, and $\mathscr{A}_3$ and the side length $\ell = \sqrt{2}/2$, and the maximum value corresponds to an equilateral triangle with vertices $\mathscr{A}_1$, $\mathscr{A}_2$, and $\mathscr{A}_3$ and the side length $\ell = 1$; see Fig. 16.1a. The illustration of the states by the triangle and Malevich's squares geometry was called *the quantum suprematism picture of spin states*; see Fig. 16.1b.

The quantumness of states is described by the inequality constraint (16.34). If the probabilities p_1, p_2, and p_3 correspond to the statistics of three classical dihotomic variables (three classical coin positions "UP" and "DOWN"), the maximum value

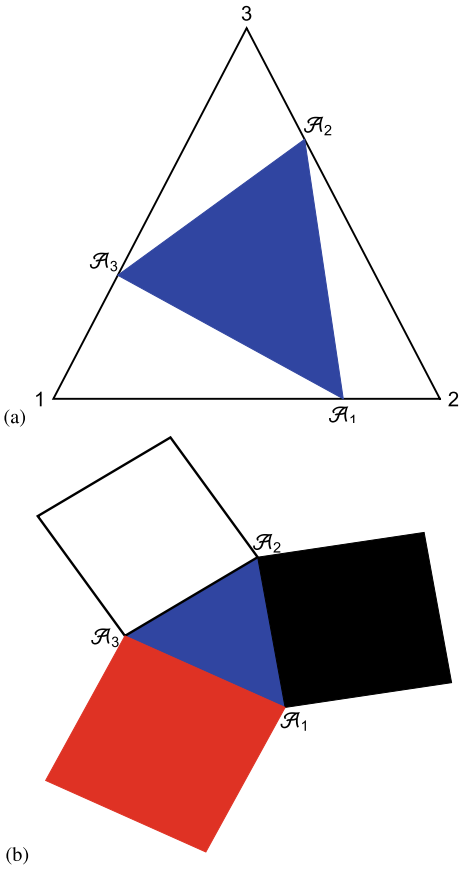

Fig. 16.1 Equilateral triangle constructed of three simplexes and vertices $\mathscr{A}_1$, $\mathscr{A}_2$, and $\mathscr{A}_3$ (**a**) and Triada of Malevich's squares illustrated the qubit state (**b**)

of Malevich's squares $S^{\mathrm{cl}}_{\max} = 6$ since, in this case, the triangle $\mathscr{A}_1\mathscr{A}_2\mathscr{A}_3$ coincides with the initial equilateral triangle with the side length equal to $\sqrt{2}$.

Thanks to the introduced H-representation of qubit state, there exists the map of the qubit density matrix onto its H-tomographic symbol $w_{\mathbf{p}}(x_1, x_2 \mid \theta)$, where $\mathbf{p} = (p_1, p_2, p_3)$ is given by the conditional probability or the joint probability distribution $W_{\mathbf{p}}(x_1, x_2, \theta)$. We have the explicit relation of the probability vector $\mathbf{p}$ with H-tomogram; it is

$$w_{\mathbf{p}}(x_1, x_2 \mid \theta) = \frac{2\, e^{-(x_1^2+x_2^2)}}{\pi}[p_3 x_1^2 + (1-p_3)x_2^2 + \{\big(p_1 - (1/2) - i(p_2 - 1/2)\big)e^{-i\theta} + \big(p_1 - (1/2) + i(p_2 - 1/2)\big)e^{i\theta}\}x_1 x_2]. \tag{16.37}$$

For example, the H-tomogram of the pure state with the density matrix $\rho = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ reads

$$w_{\mathbf{p}}^{(z)}(x_1, x_2 \mid \theta) = \frac{2\, e^{-(x_1^2+x_2^2)}}{\pi}\, x_1^2, \tag{16.38}$$

and the H-tomogram of the state with the density matrix $\rho = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ is

$$w_{\mathbf{p}}^{(x)}(x_1, x_2 \mid \theta) = \frac{2\, e^{-(x_1^2+x_2^2)}}{\pi}\left(\frac{x_1^2 + x_2^2}{2} + x_1 x_2 \cos\theta\right). \tag{16.39}$$

The superposition principle of two pure states yields the nonlinear addition rule of the probability distributions (16.38) and (16.39) analogous to the one considered in [14, 15].

The mean value of an observable $\hat{A}$ is defined by the formula

$$\mathrm{Tr}\left(\hat{A}\hat{\rho}\right) = \iint_0^{2\pi} w(x_1, x_2 \mid \theta) w_A^{(d)}(x_1, x_2, \theta)\, dx_1\, dx_2\, d\theta, \tag{16.40}$$

where the dual symbol [24, 28] of the observable $\hat{A}$ is calculated, in view of the quantizer $\hat{D}(x_1, x_2; \theta)$,

$$w_A^{(d)}(x_1, x_2, \theta) = \mathrm{Tr}\left(\hat{A}\hat{D}(x_1, x_2; \theta)\right). \tag{16.41}$$

If the matrix $A_{mm'}$ of the observable $\hat{A}$ is given, the dual symbol reads

$$\begin{aligned} w_A^{(d)}(x_1, x_2, \theta) = \frac{1}{4\pi}\big\{&A_{1/2\ 1/2}[H_2(x_1)/2] + A_{1/2\ -1/2} e^{i\theta} H_1(x_1) H_1(x_2) \\ &+ A_{-1/2\ 1/2} e^{-i\theta} H_1(x_1) H_1(x_2) + A_{-1/2\ -1/2}[H_2(x_2)/2]\big\}. \end{aligned} \tag{16.42}$$

We point out that the dual symbol of the density operator $\hat{\rho}$ is not a probability distribution.

16.7 Generic Qudit State in the H-Representation

The tomogram $w^{(s)}(x_1, x_2 \mid \theta)$ for an arbitrary spin-s state reads [9]

$$\begin{aligned} w_{(s)}(x_1, x_2 \mid \theta) = &\frac{e^{-(x_1^2+x_2^2)}}{4^s \pi} \sum_{m_1, m_2 = -s}^{s} \rho_{m_1 m_2}^{(s)}\, e^{-i(m_1 - m_2)\theta} \\ &\times \frac{H_{s+m_1}(x_1)\, H_{s+m_2}(x_1)\, H_{s-m_1}(x_2)\, H_{s-m_2}(x_2)}{\sqrt{(s+m_1)!\,(s+m_2)!\,(s-m_1)!\,(s-m_2)!}}. \end{aligned} \tag{16.43}$$

The joint probability distribution of three random variables

$$W^{(s)}(x_1, x_2, \theta) = w^{(s)}(x_1, x_2 \mid \theta)\, \Pi(\theta), \tag{16.44}$$

where $1 \leq \Pi(\theta) \leq 0$ and $\int_0^{2\pi} \Pi(\theta)\, d\theta = 1$, provides three probability distributions

$$W_{12}(x_1, x_2) = \int_0^{2\pi} W^{(s)}(x_1, x_2, \theta)\, d\theta, \tag{16.45}$$

$$W_{23}(x_2, \theta) = \int W^{(s)}(x_1, x_2, \theta)\, dx_1, \tag{16.46}$$

$$W_2(x_2) = \iint_0^{2\pi} W^{(s)}(x_1, x_2, \theta)\, dx_1\, d\theta. \tag{16.47}$$

These marginal probability distributions satisfy the strong subadditivity condition, which is a new inequality depending on the matrix elements of the density matrix of arbitrary spin states; it is

$$\begin{aligned} &-\iint_0^{2\pi} W^{(s)}(x_1, x_2, \theta) \ln W^{(s)}(x_1, x_2, \theta)\, dx_1\, dx_2\, d\theta - \int W_2(x_2) \ln W_2(x_2)\, dx_2 \\ &\leq -\int W_{12}(x_1, x_2) \ln W_{12}(x_1, x_2)\, dx_1\, dx_2 - \iint_0^{2\pi} W_{23}(x_2, \theta) \ln W_{23}(x_2, \theta)\, dx_2\, d\theta. \end{aligned} \tag{16.48}$$

This inequality is valid for an arbitrary probability distribution $\Pi(\theta)$, including $\Pi(\theta) = (2\pi)^{-1}$.

The other new entropic inequality, namely, the subadditivity condition reads

$$\begin{aligned} &-\iint_0^{2\pi} W^{(s)}(x_1, x_2, \theta) \ln W^{(s)}(x_1, x_2, \theta)\, dx_1\, dx_2\, d\theta \\ &\leq -\int W_1^{(s)}(x_1) \ln W_1^{(s)}(x_1)\, dx_1 - \iint_0^{2\pi} W_{23}^{(s)}(x_2, \theta) \ln W_{23}^{(s)}(x_2, \theta)\, dx_2\, d\theta, \end{aligned} \tag{16.49}$$

where the marginal probability distribution $W_1^{(s)}(x_1)$ is

$$W_1^{(s)}(x_1) = \iint_0^{2\pi} W^{(s)}(x_1, x_2, \theta)\, dx_2\, d\theta. \tag{16.50}$$

The case of equality in (16.49) corresponds to the absence of correlations of a random variable x_1 and a pair of two random variables x_2 and θ.

In the case of $\Pi(\theta) = (2\pi)^{-1}$, the marginal probability distribution $W_{12}(x_1, x_2)$ has the form

$$W_{12}(x_1, x_2) = \frac{e^{-(x_1^2+x_2^2)}}{4^s\pi} \sum_{m-s}^{s} \rho_{mm} \frac{H^2_{s+m}(x_1)}{(s+m)!} \frac{H^2_{s-m}(x_2)}{(s-m)!}. \tag{16.51}$$

This probability distribution of two random variables is expressed in terms of diagonal elements of the spin density matrix ρ_{mm} and optical tomogram of energy-level states of two-mode harmonic oscillator. The symplectic tomogram of the two-mode harmonic oscillator reads [19, 29, 30]

$$w(X_1, X_2 \mid \mu_1, \nu_1, \mu_2, \nu_2) = \mathrm{Tr}\big\{ \mid n_1 n_2\rangle\langle n_1 n_2 \mid \times\delta\big(X_1 - \mu_1\hat{q}_1 - \nu_1\hat{p}_1\big)\,\delta\big(X_2 - \mu_2\hat{q}_2 - \nu_2\hat{p}_2\big)\big\}, \tag{16.52}$$

where the energy levels $E_{n_1n_2} = (n_1 + n_2 + 1)$; $n_1, n_2 = 0, 1, 2, \ldots$, and we assume $\hbar = m = \omega = 1$. Also here, the operators $\hat{q}_1, \hat{p}_1, \hat{q}_2$, and $\hat{p}_2$ are the oscillator position and momentum operators, respectively, and μ_1, μ_2, ν_1, and ν_2 are real parameters.

The symplectic tomogram of these states is expressed in terms of the wave function $\psi_{n_1n_2}(X_1, X_2)$ as follows:

$$w_{n_1n_2}(X_1, X_2 \mid \mu_1, \nu_1, \mu_2, \nu_2) = \frac{1}{\sqrt{(\mu_1^2 + \nu_1^2)(\mu_2^2 + \nu_2^2)}} \left| \psi_{n_1n_2}\left(\frac{X_1}{\sqrt{\mu_1^2 + \nu_1^2}}, \frac{X_2}{\sqrt{\mu_2^2 + \nu_2^2}} \right) \right|^2. \tag{16.53}$$

The optical tomogram can be obtained from (16.53) using the parameters $\mu_1 = \cos\theta_1$, $\nu_1 = \sin\theta_1$ and $\mu_2 = \cos\theta_2$, $\nu_2 = \sin\theta_2$; it reads

$$w_{n_1n_2}(X_1, X_2 \mid \theta_1, \theta_2) = \mathrm{Tr}\big\{ \mid n_1 n_2\rangle\langle n_1 n_2 \mid \delta\big(X_1 - \hat{q}_1\cos\theta_1 - \hat{p}_1\sin\theta_1\big) \times\delta\big(X_2 - \hat{q}_2\cos\theta_2 - \hat{p}_2\sin\theta_2\big)\big\}. \tag{16.54}$$

In view of this, we are in the position to present the optical tomographic probability distribution of the energy-level states in the explicit form:

$$w_{n_1n_2}(X_1, X_2 \mid \theta_1, \theta_2) = \frac{e^{-(X_1^2+X_2^2)}}{\pi\,(2^{n_1+n_2} n_1! n_2!)} H^2_{n_1}(X_1)\, H^2_{n_2}(X_2). \tag{16.55}$$

This tomographic probability distribution of two random oscillator positions X_1 and X_2 does not depend on angles θ_1 and θ_2. One can see that the marginal probability distributions $W_{12}(x_1, x_2)$ obtained from the H-tomogram of spin state has the form of a sum of optical tomographic probability distributions of the energy-level states of two-mode harmonic oscillator with coefficients equal to the probabilities of spin projections $m = -s, -s+1, \ldots, s$ on the z-axes of spin states with the density

matrix $\rho^{(s)}_{m_1 m_2}$. Thus, the Jordan–Schwinger map of spin states provides the possibility to connect the spin-tomography approach with oscillator tomograms by explicit formulas.

The relations obtained can also be formulated as follows.

The marginal probability distributions $W_{12}(x_1, x_2)$ obtained from the H-tomogram of spin state is equal to the mean value of "random" tomographic probability distributions of two-mode harmonic oscillator states corresponding to the energy levels $E_{n_1 n_2}$ distributed according to the diagonal matrix elements of the spin-state density matrix. Such kinds of correlations can be found also using the tomographic approach to the field theory developed in [29, 30].

16.8 Conclusions

To conclude, we point out our main results presented in this paper.

We reviewed the Jordan–Schwinger map and the quantum suprematism approach to illustrate the qubit states by Triadas of Malevich's squares. Using the representation of qubit states in terms of Hermite polynomials and three probabilities of spin projections $m = +1/2$ onto three perpendicular directions, we obtained new entropic inequalities for the probabilities identified with qubit states.

We calculated the dual symbol of an arbitrary qubit observable in the H-representation of the states and derived the expression for the means of observables in an explicit form.

The approach to quantum observables considered in [31] as classical-like random variables and the triangle geometry of the hydrogen atom [32, 33] associated with the $O(4, 2)$ group, using the quantum suprematism picture, can be applied to the other vibrational systems, including nonlinear f-oscillators [34].

We dedicate this paper to Alberto Ibort, our big friend and collaborator in connection with his 60th years birthday.

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Chapter 17
On Sympletic Lifts of Actions for Complete Lagrangian Fibrations

Juan Carlos Marrero and Edith Padrón

Abstract In this note we discuss symplectic lifts of actions for a complete Lagrangian fibration. Firstly, we describe the symplectic cotangent lifts of a G-action on a manifold Q in terms of 1-cocycles in the cohomology of G induced by the action with values in the space of closed 1-forms on Q. After this, we consider the general case of complete Lagrangian fibrations.

Mathematics Subject Classification (2010) 53D05 · 53D12 · 70G45 · 70H15.

17.1 Introduction

A Lagrangian fibration π is a surjective submersion with total space a symplectic manifold M and such that the fibers of π are Lagrangian submanifolds of M. It is well-known that Lagrangian fibrations are closely related with the theory of Arnold-Liouville of completely integrable systems [1, 2] and this is a good motivation for the discussion of such objects. The typical example of a Lagrangian fibration is the canonical projection from the cotangent bundle T^*Q of a manifold Q over Q. This Lagrangian fibration is complete because the vertical lift of every 1-form on Q is a complete vector field on T^*Q (see, for instance, [5] for the definition of the vertical lift of a 1-form to the cotangent bundle).

Dedicated to our friend Alberto Ibort on the occasion of his 60th birthday.

J. C. Marrero (✉) · E. Padrón
Unidad asociada ULL-CSIC, Geometría Diferencial y Mecánica Geométrica
Departamento de Matemática, Estadística e I.O., Universidad de la Laguna, La Laguna, 38071 Tenerife, Canary Islands, Spain
e-mail: jcmarrer@ull.edu.es

E. Padrón
e-mail: mepadron@ull.edu.es

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_17

The vertical lift to the total space of an arbitrary Lagrangian fibration π of a 1-form on the base space is also a well-defined vector field and, by analogy with the case of the cotangent bundle, π is said to be complete if such vector fields are complete.

Every complete Lagrangian fibration $\pi : M \to Q$ defines a new complete Lagrangian fibration with total space the quotient T^*Q/Λ and base space Q, where $\Lambda = \bigcup_{q \in Q} \Lambda_q$ is a Lagrangian submanifold of T^*Q and Λ_q is a discrete subgroup of the additive group of T^*_qQ. In fact, T^*_qQ/Λ_q is (non-canonically) diffeomorphic to the Lagrangian fiber $\pi^{-1}(q)$. However, M and T^*Q/Λ are not, in general, globally isomorphic. Under a strong hyphothesis, the presence of a global Lagrangian section of the fibration $\pi : M \to Q$, one may prove that there exists a global fiber-preserving symplectomorphism between M and T^*Q/Λ. The Lagrangian fibration $\widetilde{\pi}_Q : T^*Q/\Lambda \to Q$ is called the symplectic reference of $\pi : M \to Q$ (for more details, see [4]).

On the other hand, it is well-known that the standard example of a sympletic action on the cotangent bundle of a manifold Q is the cotangent lift of an action ϕ on Q. This action is very interesting from a mathematical and physical point of view. In fact, it plays an important role in the study of symmetric Hamiltonian systems (see, for instance, [1, 6–8]).

The aim of this note is to discuss symplectic lifts of actions for complete Lagrangian fibrations. First of all, we consider the particular case when the Lagrangian fibration is the standard projection $\pi_Q : T^*Q \to Q$. In such a case, we prove that every symplectic lift of a G-action ϕ on Q is the composition of the cotangent lift of ϕ with a translation. This translation is given by a 1-cocycle in the cohomology of G induced by ϕ with values in the space of closed 1-forms on Q. Moreover, the symplectic action is completely determined, up to isomorphism, by the cohomology class of the 1-cocycle. In the general case of an arbitrary complete Lagrangian fibration $\pi : M \to Q$, we prove similar results using the symplectic reference $\widetilde{\pi}_Q : T^*Q/\Lambda \to Q$ of $\pi : M \to Q$.

The note is structured as follows. In Sect. 17.2, we discuss the symplectic lifts of actions for the standard Lagrangian fibration $\pi_Q : T^*Q \to Q$ and, in Sect. 17.3, we obtain the corresponding results for an arbitrary complete Lagrangian fibration.

17.2 Symplectic Cotangent Lifts of Actions on a Manifold

Let Q be a manifold of dimension n. We denote by θ_Q the Liouville 1-form, by $\omega_Q = -d\theta_Q$ the canonical symplectic structure on the cotangent bundle T^*Q and by $\pi_Q : T^*Q \to Q$ the corresponding projection of T^*Q on Q.

In addition, we suppose that we have a left action $\phi : G \times Q \to Q$ of a Lie group G on Q. Denote by $T^*\phi : G \times T^*Q \to T^*Q$ the cotangent lift action given by

$$(T^*\phi)_g \alpha_q := T^*_{\phi_g(q)} \phi_{g^{-1}}(\alpha_q), \qquad \text{for } g \in G \text{ and } \alpha_q \in T^*_qQ.$$

The cotangent lift $T^*\phi$ of the action $\phi : G \times Q \to Q$ is a fiberwise symplectic action, i.e.

$$\pi_Q \circ (T^*\phi)_g = \phi_g \circ \pi_Q, \text{ and } (T^*\phi)_g^* \omega_Q = \omega_Q, \quad \text{for all } g \in G.$$

Now, we ask about if it is possible to consider other symplectic actions on (T^*Q, ω_Q) which fiber on ϕ.

It is well-known that a diffeomorphism $F : T^*Q \to T^*Q$ on T^*Q preserves the Liouville 1-form θ_Q if and only if there is a diffeomorphim $f : Q \to Q$ such that $F = T^*f$ (see Proposition 6.3.2 in [7]). So, if F is a fiber-preserving diffeomorphism then F is the identity.

Moreover, we may prove the following result.

Proposition 1 *Let $F : T^*Q \to T^*Q$ be a diffeomorphism which is fibered over the identity. The following statements are equivalent:*

(i) F is symplectic with respect to the canonical symplectic structure ω_Q on T^*Q.
(ii) There exists a unique closed 1-form α on Q such that F is just the fiber translation $t_\alpha : T^*Q \to T^*Q$ by α, that is,

$$t_\alpha(\gamma_q) = \gamma_q + \alpha(q), \quad \textit{for all } \gamma_q \in T_q^*Q.$$

Proof Suppose that F is the fiber translation t_α by a 1-form α on Q. Then, a direct proof using local coordinates allows to obtain the following formula

$$F^*\omega_Q = t_\alpha^*\omega_Q = \omega_Q - \pi_Q^*(d\alpha). \tag{17.1}$$

Thus, if α is closed,

$$F^*\omega_Q = \omega_Q.$$

Conversely, if (i) is satisfied, we can consider a 1-form $\alpha \in \Omega^1(Q)$ given by

$$\alpha(q) = F(\gamma_q) - \gamma_q,$$

where γ_q is an arbitrary element of T_q^*Q. We will see that, for each $q \in Q$, this definition does not depend on the choice of $\gamma_q \in T_q^*Q$, or equivalently, the linear map $T_{\gamma_q}(F - id_{T^*Q})$ is null on vertical vectors. Note that, since F is fibered over the identity, the map $F - id_{T^*Q}$ is well-defined.

Let λ be a 1-form on Q, then its vertical lift $X_{\pi_Q^*\lambda}$ is a vector field on T^*Q which is characterized in terms of the canonical symplectic structure on T^*Q as follows (see [5])

$$i_{X_{\pi_Q^*\lambda}}\omega_Q = \pi_Q^*\lambda. \tag{17.2}$$

In fact, we have that (see [5])

$$X_{\pi_Q^*\lambda}(\beta_q) = \frac{d}{dt}_{|t=0}(\beta_q + t\lambda(q)) \text{ for } \beta_q \in T_q^*Q. \tag{17.3}$$

This implies that the vertical bundle $V_{\beta_q}\pi_Q$ of π_Q at the point $\beta_q \in T_q^*Q$ is

$$V_{\beta_q}\pi_Q = \{X_{\pi_Q^*\lambda}(\beta_q)/\lambda \in \Omega^1(Q)\}.$$

Moreover, if f is a fiberwise linear function on T^*Q then there exists a vector field Y on Q such that $f = \widehat{Y}$, that is,

$$f(\beta_q) =< \beta_q, Y(q) >, \text{ for } \beta_q \in T_q^*Q, \tag{17.4}$$

and one may prove that

$$X_{\pi_Q^*\lambda}(\widehat{Y}) = \lambda(Y) \circ \pi_Q. \tag{17.5}$$

Now, from (17.2) and using that F is symplectic, we have that

$$i_{X_{\pi_Q^*\lambda}}F^*(\omega_Q) = i_{X_{\pi_Q^*\lambda}}\omega_Q = \pi_Q^*\lambda = (\pi_Q \circ F)^*\lambda = F^*(\pi_Q^*\lambda) = F^*(i_{X_{\pi_Q^*\lambda}}\omega_Q).$$

As a consequence, using the non-degeneracy of ω_Q, we deduce that

$$T_{\gamma_q}F(X_{\pi_Q^*\lambda}(\gamma_q)) = X_{\pi_Q^*\lambda}(F(\gamma_q)) \text{ for all } \gamma_q \in T_q^*Q. \tag{17.6}$$

On the other hand, since $\pi_Q \circ F = \pi_Q$ then $T_{\gamma_q}(F - id_{T^*Q})(X_{\pi_Q^*\lambda}(\gamma_q))$ is a vertical vector, so it is characterized by its value on fiberwise linear functions $f \in C^\infty(T^*Q)$. Thus, using (17.5) and (17.6), we have that

$$T_{\gamma_q}(F - id_{T^*Q})(X_{\pi_Q^*\lambda}(\gamma_q))(f) = X_{\pi_Q^*\lambda}(F(\gamma_q))(f) - X_{\pi_Q^*\lambda}(\gamma_q)(f) = 0,$$

which proves the proposition.

Now, suppose that we have an arbitrary symplectic action $\Phi : G \times T^*Q \to T^*Q$ such that projects on an action $\phi : Q \to Q$, i.e. the following diagram commutes

$$\begin{array}{ccc} T^*Q & \xrightarrow{\Phi_g} & T^*Q \\ \downarrow{\scriptstyle \pi_Q} & & \downarrow{\scriptstyle \pi_Q} \\ Q & \xrightarrow{\phi_g} & Q \end{array}$$

and $\Phi_g^*(\omega_Q) = \omega_Q$, for all $g \in G$. We ask about how are these symplectic actions on T^*Q. The following result gives an answer to this question.

Proposition 2 *Let $\Phi : G \times T^*Q \to T^*Q$ be a symplectic action of a Lie group G on (T^*Q, ω_Q) whose projection on Q is the action $\phi : G \times Q \to Q$. Then, there exists a differentiable map $A : G \times Q \to T^*Q$ such that*

1. *A is fibered on Q, i.e. $\pi_Q \circ A = pr_2$, where $pr_2 : G \times Q \to Q$ is the canonical projection on the second factor.*
2. *For each $g \in G$, the 1-form A_g on Q is closed.*
3. *The action Φ is given by*

$$\Phi_g = (T^*\phi)_g \circ t_{A(g)}, \text{ for all } g \in G. \tag{17.7}$$

In particular, Φ is an affine action. Moreover, Φ is linear if and only if Φ is the cotangent lift $T^*\phi$ of ϕ.

Proof Let g be an element of the Lie group G. The map $F_g = (T^*\phi)_{g^{-1}} \circ \Phi_g$ satisfies the hypothesis of Proposition 1. Thus, there exists a unique closed 1-form A_g on Q such that $\Phi_g = (T^*\phi)_g \circ t_{A(g)}$.

Therefore, if $\Omega^1_c(Q)$ denotes the set of closed 1-forms on Q, every symplectic fiberwise action is affine and it induces a map $A : G \to \Omega^1_c(Q)$ satisfying (17.7) but, does each one of these maps induces an affine symplectic fiberwise action? The following result give us the necessary and sufficient conditions on the map $A : G \to \Omega^1_c(Q)$ to ensure that the map $\Phi^A : G \times T^*Q \to T^*Q$ related with A by (17.7) is a symplectic action. Previously, we introduce the following cohomology complex induced by the action ϕ (see, for instance, [3]):

– A n-cochain is a map $A : G \times \overset{n}{\ldots} \times G \to \Omega^1(Q)$ and $C^n(G, \Omega^1(Q))$ denotes the set of the n-cochains. The 0-cochains are the 1-forms on Q.
– The coboundary operator $\delta_\phi : C^n(G, \Omega^1(Q)) \to C^{n+1}(G, \Omega^1(Q))$ is given by

$$\begin{aligned}(\delta_\phi A)(g_1, \ldots, g_{n+1}) = &(-1)^{n+1} A(g_2, \ldots, g_{n+1}) + \\ &+ \sum_{i=1}^{n} (-1)^{n+i+1} A(g_1, \ldots, g_{i-1}, g_i \cdot g_{i+1}, \ldots, g_{n+1}) + \\ &+ \phi^*_{g_{n+1}}(A(g_1, \ldots, g_n)).\end{aligned}$$

Since the exterior differential is linear and commutes with the pull back, then the sets $C^n(G, \Omega^1_c(Q))$ of the n-cochains with values in the closed 1-forms on Q define a subcomplex of $(C^\bullet(G, \Omega^1(Q)), \delta_\phi)$. We denote by $H^k(G, \phi, \Omega^1_c(Q))$ the corresponding cohomology groups. We will see that the first cohomology group $H^1(G, \phi, \Omega^1_c(Q))$ allows to classify the symplectic actions on T^*Q which project on ϕ.

Theorem 1 *Let $\phi : G \times Q \to Q$ be an action of the Lie group G on a manifold Q and A be a map from G to $\Omega^1(Q)$. Then,*

1. *The map $\Phi^A : G \times T^*Q \to T^*Q$ given by $\Phi^A_g = (T^*\phi)_g \circ t_{A(g)}$ is an action if and only if A is a one-cocycle in the cohomology complex $(C^\bullet(G, \Omega^1(Q)), \delta_\phi)$.*
2. *Φ^A is also symplectic if and only if $A(g)$ is a closed 1-form on Q, for all $g \in G$, i.e. A is a one-cocycle in the cohomology subcomplex $(C^\bullet(G, \Omega^1_c(Q)), \delta_\phi)$.*

Proof The left action condition $\Phi^A_{gh} = \Phi^A_g \circ \Phi^A_h$ is equivalent to the relation

$$(T^*\phi)_{gh}(A(gh)(q)) = (T^*\phi)_{gh}(A(h)(q)) + (T^*\phi)_g(A(g)(\phi_h(q))).$$

If we apply $(T^*\phi)_{(gh)^{-1}}$ in the previous equality, then we have

$$A(gh) = A(h) + \phi_h^*(A(g)), \qquad \forall\, g, h \in G.$$

Note that this last condition implies that $A(e) = 0$, where e is the identity element of G. Therefore, Φ^A is an action if and only if A is a one-cocycle in the cohomology complex $(C^\bullet(G, \Omega^1(Q)), \delta_\phi)$.

On the other hand, using (17.1) and the symplectic character of the cotangent lift action, we deduce

$$\begin{aligned}(\Phi^A_g)^*(\omega_Q) &= t^*_{A(g)}((T^*\phi)^*_g\omega_Q) = t^*_{A(g)}\omega_Q \\ &= \omega_Q - \pi_Q^*(d(A(g))).\end{aligned}$$

Thus, Φ^A_g is symplectic if and only if $A(g)$ is a closed 1-form on Q, for all $g \in G$.

Note that the previous results give us a relation between symplectic actions on (T^*Q, ω_Q) whose projection on Q is $\phi : G \times Q \to Q$ and one-cocycles in the cohomology complex $(C^\bullet(G, \Omega^1_c(Q)), \delta_\phi)$. Using these facts, we will see in the following theorem that the first cohomology group $H^1(G, \phi, \Omega^1_c(Q))$ of this complex allows to give a classification of these symplectic actions on (T^*Q, ω_Q).

Theorem 2 *Let $\phi : G \times Q \to Q$ be an action of a Lie group G on a manifold Q. If $A, B : G \to \Omega^1_c(Q)$ are two one-cocycles in the cohomology complex $(C^\bullet(G, \Omega^1_c(Q)), \delta_\phi)$, and Φ^A and Φ^B their respective affine symplectic actions on (T^*Q, ω_Q), then exists a symplectomorphism $F : T^*Q \to T^*Q$ such that*

$$\pi_Q \circ F = \pi_Q \text{ and} \tag{17.8}$$

$$F \circ \Phi^A_g = \Phi^B_g \circ F, \text{ for all } g \in G \tag{17.9}$$

if and only if $[A] = [B] \in H^1(G, \phi, \Omega^1_c(Q))$.

Proof Suppose that $F : T^*Q \to T^*Q$ is a symplectomorphism which satisfies (17.8) and (17.9). Then, using Proposition 1, we deduce that there exists a closed 1-form α on Q such that $F = t_\alpha$. Since $t_\alpha \circ \Phi^A_g = \Phi^B_g \circ t_\alpha$, we have that

$$(T^*\phi)_g(\gamma_q + A(g)(q) + \alpha(\phi_g(q))) = (T^*\phi)_g(\gamma_q + B(g)(q) + \alpha(q)),$$

for all $\gamma_q \in T^*_qQ$. Thus, we deduce

$$(A - B)(g) = \alpha - \phi_g^*\alpha = \delta_\phi(-\alpha)(g),$$

that is, $[A] = [B]$.

Conversely, if $[A] = [B]$, then there exists a closed 1-form α on Q such that $(A - B)(g) = \delta_\phi(\alpha)(g) = \phi_g^*\alpha - \alpha$. Thus, $F = t_{-\alpha}$ satisfies the conditions of the theorem.

Example 1 (**The Heisenberg group**) Let $Q = \mathbb{R}^3 \cong \mathbb{R}^2 \times \mathbb{R}$ be the Heisenberg group endowed with the group law

$$(x, y, t) \cdot (x', y', t') = (x + x', y + y', t + t' + xy'), \quad \text{for all } (x, y, t), (x', y', t') \in \mathbb{R}^3.$$

We consider the action $\phi : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3$ defined by the group operation. The cotangent lift action $T^*\phi$ is

$$(T^*\phi)_{(x_0,y_0,t_0)}(x, y, t, \alpha_1, \alpha_2, \alpha_3) = (x + x_0, y + y_0, t + t_0 + x_0 y, \alpha_1, \alpha_2 - x_0\alpha_3, \alpha_3).$$

Here we have identified $T^*\mathbb{R}^3 \cong \mathbb{R}^6$.

Let $A : \mathbb{R}^3 \to \Omega_c^1(\mathbb{R}^3)$ be the one-cocycle

$$A(x_0, y_0, t_0) = x_0^2 dy + 2x_0 dt, \text{ for all } (x_0, y_0, t_0) \in \mathbb{R}^3.$$

Note that

$$A(x_0 + x_1, y_0 + y_1, t_0 + t_1 + x_0 y_1) = A(x_1, y_1, t_1) + \phi^*_{(x_1,y_1,t_1)} A_{(x_0,y_0,t_0)}.$$

Suppose that A is a coboundary in the cohomogy complex $(C^\bullet(\mathbb{R}^3, \Omega_c^1(\mathbb{R}^3)), \delta_\phi)$. Then there exists a closed 1-form $\alpha = \alpha_1 dx + \alpha_2 dy + \alpha_3 dt$ such that $A(x_0, y_0, t_0) = \phi^*_{(x_0,y_0,t_0)}\alpha - \alpha$ for all $(x_0, y_0, t_0) \in \mathbb{R}^3$, i.e.

$$\begin{aligned} 0 &= \alpha_1 \circ \phi_{(x_0,y_0,t_0)} - \alpha_1, \\ x_0^2 &= \alpha_2 \circ \phi_{(x_0,y_0,t_0)} + x_0\alpha_3 \circ \phi_{(x_0,y_0,t_0)} - \alpha_2, \\ 2x_0 &= \alpha_3 \circ \phi_{(x_0,y_0,t_0)} - \alpha_3. \end{aligned}$$

At the point $(0, 0, 0) \in \mathbb{R}^3$ we have that

$$\begin{aligned} \alpha_1(x_0, y_0, t_0) &= \alpha_1(0, 0, 0), \\ \alpha_2(x_0, y_0, t_0) &= x_0^2 - x_0\alpha_3(0, 0, 0) + \alpha_2(0, 0, 0), \\ \alpha_3(x_0, y_0, t_0) &= 2x_0 + \alpha_3(0, 0, 0). \end{aligned}$$

On the other hand, since α is closed

$$\frac{\partial \alpha_1}{\partial y} - \frac{\partial \alpha_2}{\partial x} = 0,$$

that is, $2x_0 - \alpha_3(0, 0, 0) = 0$ which it is not possible. Thus, $[A] \neq 0$.

The new symplectic action on $T^*\mathbb{R}^3$ is

$$\begin{aligned}&\Phi_{(x_0,y_0,s_0)}(x, y, t, \alpha_1, \alpha_2, \alpha_3)\\ &= (x + x_0, y + y_0, t + t_0 + x_0 y, \alpha_1, \alpha_2 - x_0^2 - x_0\alpha_3, \alpha_3 + 2x_0),\end{aligned}$$

and $(T^*\mathbb{R}^3, \Phi)$ is not symplectomorphic to $(T^*\mathbb{R}^3, T^*\phi)$.

17.3 Symplectic Lifts of Actions on a Complete G-Lagrangian Fibration

The cotangent projection $\pi_Q : T^*Q \to Q$ of a manifold Q has a special property: for all $q \in Q$, its fiber T_q^*Q at q is a Lagrangian submanifold of T^*Q, that is, $\pi_Q : T^*Q \to Q$ is a Lagrangian fibration. In this section we will extend the previous results to this kind of fibrations (with certain topological restrictions). In order to do this, we recall some notions and properties about Lagrangian fibrations (for more details, see [4]).

A fiber bundle $\pi : M \to Q$, with total space a symplectic manifold (M, ω), is called a *Lagrangian fibration* if its fiber $\pi^{-1}(q)$ is a Lagrangian submanifold of M, for all $q \in Q$, that is,

$$\ker T_x\pi = (\ker T_x\pi)^{\omega}, \quad \text{for all } x \in \pi^{-1}(q), \tag{17.10}$$

where $(\ker T_x\pi)^{\omega} = \{v \in T_xM / \omega_x(v, u) = 0 \text{ for all } u \in \ker T_x\pi\}$ is the symplectic orthogonal subspace of $\ker T_x\pi$.

Consider (M, Q, π, ω) a Lagrangian fibration. Given a 1-form α on Q, denote by $X_{\pi^*\alpha}$ the vertical vector field on M which is characterized by the following condition

$$i_{X_{\pi^*\alpha}}\omega = \pi^*\alpha. \tag{17.11}$$

Note that (17.10) implies that $X_{\pi^*\alpha}$ is a vertical vector field with respect to π (in fact, using (17.10), we deduce that the vertical bundle to π is generated by the vector fields $X_{\pi^*\alpha}$, with α a 1-form on Q). So, if $F_t^{X_{\pi^*\alpha}} : M \to M$ is the flow of $X_{\pi^*\alpha}$ at the time t, then $\pi \circ F_t^{X_{\pi^*(\alpha)}} = \pi$ and one can prove that

$$\frac{d}{dt}[(F_t^{X_{\pi^*\alpha}})^*(\omega)] = (F_t^{X_{\pi^*\alpha}})^*(\mathcal{L}_{X_{\pi^*\alpha}}\omega) = (F_t^{X_{\pi^*\alpha}})^*(\pi^*(d\alpha)) = \pi^*(d\alpha).$$

Therefore,

$$(F_t^{X_{\pi^*\alpha}})^*\omega = \omega + t\pi^*(d\alpha). \tag{17.12}$$

We will say that the Lagrangian fibration (M, Q, π, ω) is *complete* if the vector field $X_{\pi^*\alpha}$ is complete, for all $\alpha \in \Omega^1(Q)$. In such a case, this vector field can be integrated up to time 1 to give the map

$$\begin{aligned} \mu : \Omega^1(Q) \times M &\to M \\ (\alpha, x) &\mapsto F_1^{X_{\pi^*\alpha}}(x). \end{aligned} \tag{17.13}$$

In fact, one can check that (see [4])

- μ is an action: $\mu(\alpha + \beta, x) = \mu(\alpha, \mu(\beta, x))$,
- μ is π-fibered: $\pi(\mu(\alpha, x)) = \pi(x)$,
- $\mu(\alpha, x) = \mu(\beta, x)$ if $\alpha(\pi(x)) = \beta(\pi(x))$,
- μ is transitive on the fibers: for all $q \in Q$, if $x, x' \in \pi^{-1}(q)$, there exists a 1-form $\alpha \in \Omega^1(Q)$ such that $\mu(\alpha, x) = x'$.

Therefore, for each $q \in Q$, the action μ induces a transitive action of the abelian group T_q^*Q on the fiber $\pi^{-1}(q)$

$$\mu_q : T_q^*Q \times \pi^{-1}(q) \to \pi^{-1}(q), \qquad (\alpha_q, x) \mapsto \mu(\alpha, x), \tag{17.14}$$

where α is a 1-form on Q such that its value at q is just α_q. In general, the action μ_q is not free. For this reason we consider the isotropy subgroup Λ_q of μ_q. More explicitly,

$$\Lambda_q = \{\alpha_q \in T_q^*Q \mid \mu_q(\alpha_q, x) = x \quad \forall x \in \pi^{-1}(q)\}. \tag{17.15}$$

It can be checked that Λ_q is a discrete subgroup of T_q^*Q, T_q^*Q/Λ_q is an abelian group and $\Lambda = \cup_{q\in Q}\Lambda_q$ is a Lagrangian submanifold of T^*Q. In addition, we have the corresponding free fibered action

$$\widehat{\mu} : T^*Q/\Lambda \times M \to M.$$

On the other hand, $\widetilde{\pi}_Q : T^*Q/\Lambda \to Q$ is a Lagrangian fibration with respect the induced symplectic 2-form $\widetilde{\omega}_Q$ on the reduced space T^*Q/Λ characterized by

$$\mathrm{pr}^*\widetilde{\omega}_Q = \omega_Q, \tag{17.16}$$

where $\mathrm{pr} : T^*Q \to T^*Q/\Lambda$ is the quotient projection. Thus, $(T^*Q/\Lambda, Q, \widetilde{\pi}_Q, \widetilde{\omega}_Q)$ is a complete Lagrangian fibration. Furthermore, if the fibers of $\widetilde{\pi}_Q : T^*Q/\Lambda \to Q$ are connected and compact, then they are isomorphic to the n-torus (for more details, see [4]).

In the particular case of the Lagrangian fibration $(T^*Q, Q, \pi_Q, \omega_Q)$, the action $(\mu_Q)_q : T_q^*Q \times T_q^*Q \to T_q^*Q$ is the map $(\mu_Q)_q(\alpha_q, \beta_q) = \alpha_q + \beta_q$ and $\Lambda_q = 0$.

For the complete Lagragian fibration $(T^*Q/\Lambda, Q, \widetilde{\pi}_Q, \widetilde{\omega}_Q)$ deduced from a complete Lagrangian fibration (M, Q, π, ω), the corresponding action is

$$(\widetilde{\mu}_Q)_q : T_q^*Q \times T_q^*Q/\Lambda_q \to T_q^*Q/\Lambda_q, \quad (\widetilde{\mu}_Q)_q(\alpha_q, [\beta_q]) = [\alpha_q + \beta_q], \tag{17.17}$$

and its isotropic subgroup is just Λ_q.

Now, we will characterize the symplectomorphisms on the fiber bundle $\widetilde{\pi}_Q : T^*Q/\Lambda \to Q$. Previously, we recall the notion of *a Lagrangian section* of an arbitrary Lagrangian fibration $\pi : (M, \omega) \to Q$ like a section $\sigma : Q \to M$ of π such that $\sigma^*\omega = 0$. In the particular case of the cotangent bundle $\pi_Q : (T^*Q, \omega_Q) \to Q$, a 1-form α is Lagrangian if and if it is closed, since $\alpha^*\omega_Q = -d\alpha$.

Proposition 3 *Let $(T^*Q/\Lambda, Q, \widetilde{\pi}_Q, \widetilde{\omega}_Q)$ be the symplectic reference of a complete Lagrangian fibration (M, Q, π, ω). If $\widetilde{F} : T^*Q/\Lambda \to T^*Q/\Lambda$ is a diffeomorphism such that $\widetilde{\pi}_Q \circ \widetilde{F} = \widetilde{\pi}_Q$ then the following statements are equivalent:*

1. *$\widetilde{F}$ is a symplectomorphism, that is, $\widetilde{F}^*\widetilde{\omega}_Q = \widetilde{\omega}_Q$.*
2. *There exists a Lagrangian section $\widetilde{\sigma} : Q \to T^*Q/\Lambda$ of $\widetilde{\pi}_Q$ such that $\widetilde{F} = t_{\widetilde{\sigma}}$, where $t_{\widetilde{\sigma}} : T^*Q/\Lambda \to T^*Q/\Lambda$ is the map given by*

$$t_{\widetilde{\sigma}}([\gamma_q]) = [\gamma_q] + \widetilde{\sigma}(q), \tag{17.18}$$

for all $q \in Q$.

Proof Suppose that $\widetilde{F} = t_{\widetilde{\sigma}}$, with $\widetilde{\sigma}$ a section of $\widetilde{\pi}_Q : T^*Q/\Lambda \to Q$. Then,

$$t_{\widetilde{\sigma}}^*\widetilde{\omega}_Q = \widetilde{\omega}_Q + \widetilde{\pi}_Q^*(\widetilde{\sigma}^*\widetilde{\omega}_Q). \tag{17.19}$$

In fact, for all $\gamma_q \in T_q^*Q$, there exist a neighborhood U of q and a 1-form $\alpha : U \to T^*U$ on U such that $\alpha(q) = \gamma_q$ and

$$pr \circ \alpha = \widetilde{\sigma}_{|U}, \tag{17.20}$$

where $pr : T^*U \to T^*U/\Lambda_{|T^*U}$ is the corresponding projection. Then, we have that

$$pr \circ t_\alpha = t_{\widetilde{\sigma}_{|U}} \circ pr. \tag{17.21}$$

On the other hand, using (17.1) and (17.20), it follows that

$$t_\alpha^*\omega_Q = \omega_Q - \pi_Q^*(d\alpha) = pr^*(\widetilde{\omega}_Q + \widetilde{\pi}_Q^*(\widetilde{\sigma}^*\widetilde{\omega}_Q)).$$

From this equality, (17.16) and (17.21), we deduce that (17.19) holds. Therefore, if in addition, $\widetilde{\sigma}$ is Lagrangian, $\widetilde{F} = t_{\widetilde{\sigma}}$ is symplectic.

Conversely, if $\widetilde{F} : T^*Q/\Lambda \to T^*Q/\Lambda$ is a symplectomorphism, we define the section $\widetilde{\sigma} : Q \to T^*Q/\Lambda$ of $\widetilde{\pi}_Q : T^*Q/\Lambda \to Q$ by

$$\widetilde{\sigma}(q) = \widetilde{F}([\gamma_q]) - [\gamma_q], \qquad \text{with } \gamma_q \in T_q^*Q \text{ and } q \in Q.$$

In order to prove that $\widetilde{\sigma}$ is well defined, we will follow the proof of Proposition 1. So, we will show that for each $q \in Q$, the section $\widetilde{\sigma}$ doesn't depend of the chosen element $[\gamma_q] \in T_q^*Q/\Lambda_q$, or equivalently,

$$T_{[\gamma_q]}(\widetilde{F} - id_{T^*Q/\Lambda})(v_{[\gamma_q]}) = 0 \text{ for all } v_{[\gamma_q]} \in \ker T_{[\gamma_q]}\widetilde{\pi}_Q.$$

Let λ be a 1-form on Q and $X_{\widetilde{\pi}_Q^*\lambda}$ the vertical vector field on T^*Q/Λ of λ with respect to $\widetilde{\pi}_Q$, i.e.

$$i_{X_{\widetilde{\pi}_Q^*\lambda}}\widetilde{\omega}_Q = \widetilde{\pi}_Q^*\lambda. \tag{17.22}$$

Note that

$$X_{\widetilde{\pi}_Q^*\lambda}([\gamma_q]) = T_{\gamma_q} pr(X_{\pi_Q^*\lambda}(\gamma_q)), \text{ with } \gamma_q \in T_q^*Q, \tag{17.23}$$

where $X_{\pi_Q^*\lambda}(\gamma_q)$ is the vertical lift on T^*Q of λ with respect to $\pi_Q : T^*Q \to Q$ [(see (17.2)]. In fact, using (17.2), (17.16), (17.22) and the fact that $\widetilde{\pi}_Q \circ pr = \pi_Q$, we have

$$i_{X_{\pi_Q^*\lambda}}(pr^*\widetilde{\omega}_Q) = pr^*(i_{X_{\widetilde{\pi}_Q^*\lambda}}\widetilde{\omega}_Q).$$

So, from the non-degeneration of $\widetilde{\omega}_Q$, we deduce (17.23). It is clear that (17.23) implies that the vertical vectors $X_{\widetilde{\pi}_Q^*\lambda}([\gamma_q])$, with $\lambda \in \Omega^1(Q)$, generate the subspace $\ker T_{[\gamma_q]}\widetilde{\pi}_Q$.

Now, using that $\widetilde{F}$ is symplectic and the fact that $\widetilde{\pi}_Q \circ \widetilde{F} = \widetilde{\pi}_Q$, we deduce

$$i_{X_{\widetilde{\pi}_Q^*\lambda}}\widetilde{F}^*(\widetilde{\omega}_Q) = i_{X_{\widetilde{\pi}_Q^*\lambda}}\widetilde{\omega}_Q = \widetilde{\pi}_Q^*\lambda = (\widetilde{\pi}_Q \circ \widetilde{F})^*\lambda = \widetilde{F}^*(\widetilde{\pi}_Q^*\lambda) = \widetilde{F}^*(i_{X_{\widetilde{\pi}_Q^*\lambda}}\widetilde{\omega}_Q).$$

Then, again from the non-degeneration of $\widetilde{\omega}_Q$,

$$T_{[\gamma_q]}\widetilde{F}(X_{\widetilde{\pi}_Q^*\lambda}([\gamma_q])) = X_{\widetilde{\pi}_Q^*\lambda}(\widetilde{F}([\gamma_q])).$$

Therefore,

$$\begin{aligned} T_{[\gamma_q]}(\widetilde{F} - id_{T^*Q/\Lambda})(X_{\widetilde{\pi}_Q^*\lambda}([\gamma_q]))(\widetilde{f}) = X_{\widetilde{\pi}_Q^*\lambda}(\widetilde{F}([\gamma_q]))(\widetilde{f}) \\ -X_{\widetilde{\pi}_Q^*\lambda}([\gamma_q])(\widetilde{f}) = 0, \end{aligned} \tag{17.24}$$

for all function $\widetilde{f} : T^*Q/\Lambda \to \mathbb{R}$ such that $f = \widetilde{f} \circ pr$ is a linear function on T^*Q. Indeed, if Y is the vector field on Q associated with f defined in (17.4), then, using (17.23), we deduce that

$$X_{\widetilde{\pi}_Q^*\lambda}([\gamma_q])(\widetilde{f}) =< \lambda(q), Y(q) >= X_{\widetilde{\pi}_Q^*\lambda}(\widetilde{F}([\gamma_q]))(\widetilde{f}).$$

On the other hand, since $\widetilde{\pi}_Q \circ \widetilde{F} = \widetilde{\pi}_Q$, then $T_{[\gamma_q]}(\widetilde{F} - Id_{T^*Q/\Lambda})(X_{\widetilde{\pi}_Q^*\lambda}([\gamma_q]))$ is a vertical vector with respect $\widetilde{\pi}_Q$. In such a case, there is a vertical vector $v_{\gamma_q} \in \ker T_{\gamma_q}\pi_Q$ such that

$$T_{[\gamma_q]}(\widetilde{F} - Id_{T^*Q/\Lambda})(X_{\widetilde{\pi}_Q^*\lambda}([\gamma_q])) = T_{\gamma_q} pr(v_{\gamma_q}).$$

From (17.24), we obtain that $v_{\gamma_q}(f) = 0$ for all fiberwise linear function $f : T^*Q \to \mathbb{R}$, which implies that $v_{\gamma_q} = 0$ and, in consequence,

$$T_{[\gamma_q]}(\widetilde{F} - Id_{T^*Q/\Lambda})(X_{\widetilde{\pi}_Q^*\lambda}([\gamma_q])) = 0.$$

If the complete Lagrangian fibration (M, Q, π, ω) has a global section $\sigma : Q \to M$ then, using the action μ, we can build the following fiber bundle isomorphism from the canonical fibration $\widetilde{\pi}_Q : T^*Q/\Lambda \to Q$ to the Lagrangian fibration $\pi : M \to Q$ given by

$$\begin{array}{rcl} \varphi_\sigma : T^*Q/\Lambda & \to & M \\ \left[\alpha_q\right] & \mapsto & \mu_q(\alpha_q, \sigma(q)). \end{array} \tag{17.25}$$

This map is equivariant when we consider the additive action from T^*Q over T^*Q/Λ and the action μ on M. Moreover, using (17.12), one can prove that (see [4])

$$\varphi_\sigma^*\omega = \widetilde{\omega}_Q + \widetilde{\pi}_Q^*(\sigma^*\omega). \tag{17.26}$$

Then, if σ is Lagrangian, φ_σ is a symplectomorphism between $(T^*Q/\Lambda, Q, \widetilde{\pi}_Q, \widetilde{\omega}_Q)$ and (M, Q, π, ω).

The existence of a global Lagrangian section depends only on the triviality of Chern class of the fiber bundle $\pi : M \to B$. In fact, in [4] it is proved the following result.

Theorem 3 *The following statements are equivalent:*

1. *There exists a (symplectic) fiber bundle isomorphism between M and T^*Q/Λ.*
2. *There exists a global (Lagrangian) section $\sigma : Q \to M$ of the fiber bundle $\pi : M \to Q$.*
3. *The Chern class of the fiber bundle $\pi : M \to Q$ is null (and $\sigma^*\omega$ is an exact 2-form on Q).*

These results justify that the complete Lagrangian fibration $(T^*Q/\Lambda, Q, \widetilde{\pi}_Q, \widetilde{\omega}_Q)$ is called *the symplectic reference* or *Jacobian Lagrangian fibration* associated to the complete Lagrangian fibration (M, Q, π, ω).

Using Proposition 3 for the symplectic reference of a complete Lagrangian fibration (M, Q, π, ω), we deduce the corresponding result.

Proposition 4 *Let $\widehat{F} : M \to M$ be diffeomorphism on a complete Lagrangian fibration (M, Q, π, ω) such that $\pi \circ \widehat{F} = \pi$. Then, the following statements are equivalent:*

1. *$\widehat{F}$ is a symplectomorphism, that is, $\widehat{F}^*\omega = \omega$.*
2. *There exists a unique Lagrangian section $\widetilde{\sigma} : Q \to T^*Q/\Lambda$ of the corresponding symplectic reference $(T^*Q/\Lambda, Q, \widetilde{\pi}_Q, \widetilde{\omega}_Q)$ of (M, Q, π, ω) such that*

$$\widehat{F}(x) = \widehat{\mu}(\widetilde{\sigma}(\pi(x)), x), \text{ for all } x \in M, \tag{17.27}$$

where $\widehat{\mu} : T^*Q/\Lambda \times M \to M$ *is the free fibered action deduced from* $\mu : T^*Q \times M \to M$ *given in (17.14).*

Proof Suppose that (2) holds. Then we will prove

$$\widehat{F}^*\omega = \omega + \pi^*(\widetilde{\sigma}^*\widetilde{\omega}_Q). \tag{17.28}$$

In such a case, since $\widetilde{\sigma}^*\widetilde{\omega}_Q = 0$, then $\widehat{F}$ is symplectic.

Let x be an arbitrary point of M. Then, there exists an open neighborhood U of $q = \pi(x)$ and a local section $\sigma : U \to \pi^{-1}(U)$ of π such that the map $\varphi_\sigma : T^*U/\Lambda_{|U} \to \pi^{-1}(U)$ defined as in (17.25) is a fiber bundle isomorphism and

$$\varphi_\sigma^*\omega = \widetilde{\omega}_Q + \widetilde{\pi}_Q^*(\sigma^*\omega), \tag{17.29}$$

[see (17.26)]. Denote by $\widetilde{F} = \varphi_\sigma^{-1} \circ \widehat{F} \circ \varphi_\sigma$. Then, for all $q' \in U$ and $\alpha_{q'} \in T^*_{q'}U$,

$$\begin{aligned}\widehat{\mu}(\widetilde{F}([\alpha_{q'}]), \sigma(q')) &= \varphi_\sigma(\widetilde{F}([\alpha_{q'}])) = \widehat{F}(\varphi_\sigma([\alpha_{q'}])) \\ &= \widehat{\mu}(\widetilde{\sigma}(\pi(\varphi_\sigma([\alpha_{q'}]))), \varphi_\sigma([\alpha_{q'}])) \\ &= \widehat{\mu}(\widetilde{\sigma}(q'), \widehat{\mu}([\alpha_{q'}], \sigma(q')) = \widehat{\mu}(\widetilde{\sigma}(q') + [\alpha_{q'}], \sigma(q')).\end{aligned}$$

Now, from the free character of the action $\widehat{\mu}$ we deduce that $\widetilde{F} = t_{\widetilde{\sigma}_{|U}}$ and consequently, using (17.19) and (17.29), we have that

$$\begin{aligned}\widehat{F}^*(\omega) &= (\varphi_\sigma^*)^{-1}(\widetilde{F}^*(\varphi_\sigma^*\omega)) = (\varphi_\sigma^*)^{-1}(\widetilde{F}^*(\widetilde{\omega}_Q + \widetilde{\pi}_Q^*(\sigma^*\omega)) \\ &= (\varphi_\sigma^*)^{-1}(\widetilde{\omega}_Q + \widetilde{\pi}_Q^*(\sigma^*\omega) + \widetilde{\pi}_Q^*(\widetilde{\sigma}^*\widetilde{\omega}_Q)) = \omega + \pi^*(\widetilde{\sigma}^*\widetilde{\omega}_Q).\end{aligned}$$

Thus, (17.28) holds.

Conversely, if $\widehat{F} : M \to M$ is a symplectomorphism, with $\pi \circ \widehat{F} = \pi$, we consider the map $S : M \to T^*Q/\Lambda$ characterized by

$$\widehat{F}(x) = \widehat{\mu}(S(x), x).$$

In the following, we will prove that S is constant into $\pi^{-1}(q)$. In fact, if $x \in \pi^{-1}(q)$, there exist an open neighborhood U of q and a local section $\sigma : U \to \pi^{-1}(U)$ of π such that the map $\varphi_\sigma : T^*U/\Lambda_{|U} \to \pi^{-1}(U)$ defined by (17.25) is a fiber bundle isomorphism and

$$\varphi_\sigma^*\omega = \widetilde{\omega}_Q + \widetilde{\pi}_Q^*(\sigma^*\omega).$$

Then, using this relation and the fact that $\widehat{F}$ is symplectic, we obtain that the map $\widetilde{F} = \varphi_\sigma^{-1} \circ \widehat{F} \circ \varphi_\sigma$ is symplectic and $\widetilde{\pi}_Q \circ \widetilde{F} = \widetilde{\pi}_Q$. Now, from Proposition 3, there exists a Lagrangian section $\widetilde{\sigma} : U \to T^*U/\Lambda_{|U}$ of $\widetilde{\pi}_Q$ such that $\widetilde{F} = t_{\widetilde{\sigma}}$. In fact, $\varphi_\sigma \circ \widetilde{\sigma} = \sigma$. With a direct computation, we show that

$$\begin{aligned}\widehat{\mu}(S(y), y) &= \widehat{F}(y) = \varphi_\sigma(\widetilde{F}(\varphi_\sigma^{-1}(y))) = \widehat{\mu}(\widetilde{\sigma}(\pi(y)), \widehat{\mu}(\varphi_\sigma^{-1}(y), \sigma(\pi(y)))) \\ &= \widehat{\mu}(\widetilde{\sigma}(\pi(y)), \varphi_\sigma(\varphi_\sigma^{-1}(y))) = \widehat{\mu}(\widetilde{\sigma}(\pi(y)), y),\end{aligned}$$

for all $y \in \pi^{-1}(U)$. Thus, using the free character of the action $\widehat{\mu}$, we deduce that $S_{|U} = \widetilde{\sigma} \circ \pi$ on U.

Since S is globally defined, this proves that the Lagrangian section $\widetilde{\sigma}$ is also globally defined and $S = \widetilde{\sigma} \circ \pi$.

On the other hand, if $\widetilde{\sigma}' : Q \to T^*Q/\Lambda$ is another Lagrangian section and

$$\widehat{F}(x) = \widehat{\mu}(\widetilde{\sigma}'(\pi(x)), x), \text{ for all } x \in M,$$

then, using the free character of the action $\widehat{\mu}$, we conclude that $\widetilde{\sigma} = \widetilde{\sigma}'$.

Now, suppose that for a fibration (M, Q, π), we have actions $\phi : G \times Q \to Q$ and $\Phi : G \times M \to M$ of a Lie group G on Q and M respectively, such that π is G-equivariant, i.e. the following diagram commutes

$$\begin{array}{ccc} M & \xrightarrow{\Phi_g} & M \\ {\scriptstyle\pi}\downarrow & & \downarrow{\scriptstyle\pi} \\ Q & \xrightarrow{\phi_g} & Q \end{array}$$

for all $g \in G$. In such a case we say that (M, Q, π, ϕ, Φ) is a G-fibration.

Definition 1 Let (M, Q, π, ω) be a Labrangian fibration and Φ, ϕ be actions on M and Q respectively, such that (M, Q, π, ϕ, Φ) is a G-fibration. Then $(M, Q, \pi, \omega, \phi, \Phi)$ is a G-Lagrangian fibration if the action Φ is symplectic.

A first example of G-Lagrangian fibration is $(T^*Q, Q, \pi_Q, \omega_Q, \phi, T^*\phi)$ when we consider an action $\phi : G \times Q \to Q$ of a Lie group G on the manifold Q.

Now, fix $(M, Q, \pi, \omega, \phi, \Phi)$ a complete G-Lagrangian fibration. We can consider the action μ given by (17.13). Since Φ_g is symplectic, then, for all $\alpha \in \Omega^1(Q)$,

$$i_{(\Phi_g)_* X_{\pi^*\alpha}}\omega = (\Phi_{g^{-1}}^*)(i_{X_{\pi^*\alpha}}\omega) = (\Phi_{g^{-1}}^*)(\pi^*\alpha) = \pi^*(\phi_{g^{-1}}^*\alpha),$$

where $((\Phi_g)_* X_{\pi^*\alpha})(x) = T_{\Phi_{g^{-1}}(x)}\Phi_g(X_{\pi^*\alpha}(\Phi_{g^{-1}}(x)))$, for every $x \in M$. Therefore,

$$(T_x\Phi_g)(X_{\pi^*\alpha}(x)) = X_{\pi^*(\phi_{g^{-1}}^*\alpha)}(\Phi_g(x)),$$

that is, $X_{\pi^*\alpha}(x) = (T_{\Phi_g(x)}\Phi_{g^{-1}})(X_{\pi^*(\phi_{g^{-1}}^*(\alpha))}(\Phi_g(x)))$. Hence, we obtain the G-equivariance of the action μ, i.e.

$$\mu_{\phi_g(q)}((T^*\phi)_g\alpha_q, \Phi_g(x)) = \Phi_g(\mu_q(\alpha_q, x)), \tag{17.30}$$

for all $\alpha_q \in T_q^*Q$ and $x \in \pi^{-1}(q)$. An important consequence of this fact is that the Lagrangian submanifold Λ is G-invariant when we consider the cotangent lift action $T^*\phi$ on T^*Q. Therefore, the cotangent lifted action $T^*\phi$ induces a G-action $\widetilde{T^*\phi}$ on T^*Q/Λ and $(T^*Q/\Lambda, Q, \widetilde{\pi}_Q, \widetilde{\omega}_Q, \phi, \widetilde{T^*\phi})$ is a G-Lagrangian fibration.

Let $\widetilde{\Phi} : G \times T^*Q/\Lambda \to T^*Q/\Lambda$ be another action on T^*Q/Λ such that $(T^*Q/\Lambda, Q, \widetilde{\pi}_Q, \widetilde{\omega}_Q, \phi, \widetilde{\Phi})$ is a G-Lagrangian fibration. From (17.30) for the corresponding action $\widetilde{\mu}_Q$, we have that

$$(\widetilde{T^*\phi})_g([\alpha_q]) + \widetilde{\Phi}_g([\beta_g]) = \widetilde{\Phi}_g([\alpha_q + \beta_q]) \tag{17.31}$$

for all $\alpha_q, \beta_q \in T_q^*Q$.

Then, we define the section $\Sigma(g) : Q \to T^*Q/\Lambda$ of $\widetilde{\pi}_Q : T^*Q/\Lambda \to Q$ as follows

$$\Sigma(g)(q) = (\widetilde{T^*\phi})_{g^{-1}}(\widetilde{\Phi}_g([0_q])).$$

From (17.31), it follows that

$$\begin{aligned}\Sigma(g)(q) &= (\widetilde{T^*\phi})_{g^{-1}}(\widetilde{\Phi}_g([\gamma_q]) - (\widetilde{T^*\phi})_g([\gamma_q])),\\ &= (\widetilde{T^*\phi})_{g^{-1}}(\widetilde{\Phi}_g([\gamma_q])) - [\gamma_q],\end{aligned}$$

for $\gamma_q \in T_q^*Q$, and thus, we obtain that

$$\widetilde{\Phi}_g([\gamma_q]) = (\widetilde{T^*\phi})_g([\gamma_q]) + (\widetilde{T^*\phi})_g(\Sigma(g)(q)).$$

Therefore, since $\widetilde{\Phi}$ and $\widetilde{T^*\phi}$ are actions, we deduce that

$$\Sigma(gh) = \Sigma(h) + (\widetilde{T^*\phi})_{h^{-1}} \circ \Sigma(g) \circ \phi_h, \tag{17.32}$$

for all $g, h \in G$. This condition means that $\Sigma : G \to \mathrm{Sect}(T^*Q/\Lambda)$ is a one-cocycle in the cohomology associated with the following complex:

- A n-cochain is a map $\Sigma : G \times \overset{n}{\ldots} \times G \to \mathrm{Sect}(T^*Q/\Lambda)$. We denote by $C^n(G, \mathrm{Sect}(T^*Q/\Lambda))$ the set of the n-cochains. The set of 0-cochains is $\mathrm{Sect}(T^*Q/\Lambda)$.
- The coboundary operator

$$\delta_\phi : C^n(G, \mathrm{Sect}(T^*Q/\Lambda)) \to C^{n+1}(G, \mathrm{Sect}(T^*Q/\Lambda))$$

is given by

$$\begin{aligned}\delta_\phi \Sigma(g_1, \ldots, g_{n+1}) = (-1)^{n+1}&\Sigma(g_2, \ldots, g_{n+1}) +\\ &+ \sum_{i=1}^{n} (-1)^{n+i+1} \Sigma(g_1, \ldots, g_{i-1}, g_i g_{i+1}, \ldots, g_{n+1}) +\\ &+ (\widetilde{T^*\phi})_{g_{n+1}^{-1}} \circ \Sigma(g_1, \ldots, g_n) \circ \phi_{g_{n+1}}.\end{aligned}$$

Denote by $\mathrm{Sect}_L(T^*Q/\Lambda)$ the subspace of Lagrangian sections in the Lagrangian fibration $\widetilde{\pi}_Q : (T^*Q/\Lambda, \widetilde{\omega}_Q) \to Q$. Since $\widetilde{T^*\phi}$ is a symplectic action for

$(T^*Q/\Lambda, \widetilde{\omega}_Q)$, then $C^\bullet(G, \mathrm{Sect}_L(T^*Q/\Lambda))$ determines a subcomplex of $(C^\bullet(G, \mathrm{Sect}(T^*Q/\Lambda)), \delta_\phi)$.

In general, we have the following result.

Proposition 5 *Let (M, Q, π, ω) be a complete Lagrangian fibration and $\phi : G \times Q \to Q$ be an action on Q.*

1. *If Φ^1, Φ^2 are two symplectic lifts of $\phi : G \times Q \to Q$ then, for all $g \in G$, there exists a Lagrangian section $\Sigma(g) : Q \to T^*Q/\Lambda$ of $\widetilde{\pi}_Q : T^*Q/\Lambda \to Q$ such that*
$$\Phi^2_g(x) = \Phi^1_g(\widehat{\mu}(\Sigma(g)(\pi(x)), x)), \text{ for } x \in M, \tag{17.33}$$
where $\widehat{\mu} : T^*Q/\Lambda \times M \to M$ is the free fibered action given in (17.14).
2. *If $(M, Q, \pi, \omega, \phi, \Phi)$ is a G-Lagrangian fibration, for $\Sigma : G \to \mathrm{Sect}(T^*Q/\Lambda)$, the map $\Phi^\Sigma : G \times M \to M$ given by*
$$\Phi^\Sigma_g(x) = \Phi_g(\widehat{\mu}(\Sigma(g)(\pi(x)), x)),$$
for $x \in M$, defines an action of G on M if and only if the map Σ is a one-cocycle in the cohomology complex $(C^\bullet(G, \mathrm{Sect}(T^*Q/\Lambda)), \delta_\phi)$.
3. *In the hypothesis of (2), the action Φ^Σ is also symplectic if and only if the map Σ is a one-cocycle in the cohomology subcomplex*
$$(C^\bullet(G, \mathrm{Sect}_L(T^*Q/\Lambda)), \delta_\phi).$$

Proof (1) Consider, for all $g \in G$, the sympectomorphism $\widehat{F}_g : M \to M$ given by $\widehat{F}_g = \Phi^1_{g^{-1}} \circ \Phi^2_g$. Then, if we apply Proposition 4 to $\widehat{F}_g$, we conclude that (17.33) holds.

(2) The condition Φ^Σ is an action is equivalent with the relation

$$\Phi_h(\widehat{\mu}(\Sigma(gh)(\pi(x)), x)) = \widehat{\mu}(\Sigma(g)(\phi_h(\pi(x))), \Phi_h(\widehat{\mu}(\Sigma(h)(\pi(x)), x))).$$

Now, from (17.30), we have that

$$\begin{aligned}
&\widehat{\mu}((\widetilde{T^*\phi})_h(\Sigma(gh)(\pi(x))), \Phi_h(x)) = \\
&\widehat{\mu}(\Sigma(g)(\phi_h(\pi(x))), \widehat{\mu}((\widetilde{T^*\phi})_h(\Sigma(h)(\pi(x))), \Phi_h(x))) = \\
&\widehat{\mu}(\Sigma(g)(\phi_h(\pi(x))) + (\widetilde{T^*\phi})_h(\Sigma(h)(\pi(x))), \Phi_h(x)).
\end{aligned}$$

Therefore, the free character of $\widehat{\mu}$, implies that

$$\Sigma(gh) = \Sigma(h) + (\widetilde{T^*\phi})_{h^{-1}} \circ \Sigma(g) \circ \phi_h,$$

i.e. Σ is a one-cocyle for $(C^\bullet(G, \mathrm{Sect}(T^*Q/\Lambda), \delta_\phi)$.

(3) Let $\widehat{G}_g$ be the diffeomorphism given by

$$\widehat{G}_g(x) = \widehat{\mu}(\Sigma(\pi(x)), x), \text{ for } x \in M.$$

Then, it is clear that

$$\Phi_g^{\Sigma} = \Phi_g \circ \widehat{G}_g.$$

This, using Proposition 4, implies that $\Sigma(g)$ is a Lagrangian section for the fibration $\widetilde{\pi}_Q : T^*Q/\Lambda \to Q$.

Moreover, the cohomology $H^\bullet(G, \phi, \mathrm{Sect}_L(T^*Q/\Lambda))$ of the complex

$$(C^\bullet((G, \mathrm{Sect}_L(T^*Q/\Lambda)), \delta_\phi)$$

classifies the symplectic actions on a complete Lagrangian fibration on Q whose projection is a fixed action ϕ on Q.

Theorem 4 *Let $\phi : G \times Q \to Q$ be an action of the Lie group G on a manifold Q and (M, Q, π, ω) be a complete Lagrangian fibration on Q. Consider $\Sigma^1, \Sigma^2 : G \to \mathrm{Sect}_L(T^*Q/\Lambda)$ two one-cocycles in the cohomology complex $(C^\bullet(G, \mathrm{Sect}_L(T^*Q/\Lambda)), \delta_\phi)$, and Φ^{Σ^1} and Φ^{Σ^2} their corresponding symplectic actions of G on M. Then, there exists a symplectomorphism $\widehat{F} : M \to M$ such that*

$$\pi \circ \widehat{F} = \pi \text{ and} \tag{17.34}$$

$$\widehat{F} \circ \Phi_g^{\Sigma^1} = \Phi_g^{\Sigma^2} \circ \widehat{F}, \text{ for all } g \in G \tag{17.35}$$

if and only if $[\Sigma^1] = [\Sigma^2] \in H^1(G, \phi, \mathrm{Sect}_L(T^*Q/\Lambda))$.

Proof Suppose $\widehat{F} : M \to M$ is a symplectomorphism and that (17.34) and (17.35) hold. Then, the conditions of Proposition 4 work and therefore, there exists a Lagrangian section $\widetilde{\sigma} : Q \to T^*Q/\Lambda$ of $\widetilde{\pi}_Q$ such that $\widehat{F}(x) = \widehat{\mu}(\widetilde{\sigma}(\pi(x)), x)$. Since $\widehat{F} \circ \Phi_g^{\Sigma^1} = \Phi_g^{\Sigma^2} \circ \widehat{F}$, we have that

$$\widehat{\mu}(\widetilde{\sigma}(\phi_g(\pi(x))), \Phi_g(\widehat{\mu}(\Sigma^1(g)(\pi(x)), x))) = \Phi_g(\widehat{\mu}(\Sigma^2(g)(\pi(x)), \widehat{\mu}(\widetilde{\sigma}(\pi(x)), x))$$

for all $x \in M$.

Thus, using (17.30), it follows that

$$\widehat{\mu}(\widetilde{\sigma}(\phi_g(\pi(x))), \widehat{\mu}((\widetilde{T^*\phi})_g(\Sigma^1(g)(\pi(x))), \Phi_g(x)) = \widehat{\mu}((\widetilde{T^*\phi})_g(\Sigma^2(g)(\pi(x)) + \widetilde{\sigma}(\pi(x)), \Phi_g(x))),$$

which implies that

$$\widehat{\mu}(\widetilde{\sigma}(\phi_g(\pi(x))) + (\widetilde{T^*\phi})_g(\Sigma^1(g)(\pi(x))), \Phi_g(x)) = \widehat{\mu}((\widetilde{T^*\phi})_g(\Sigma^2(g)(\pi(x)) + (\widetilde{T^*\phi})_g(\widetilde{\sigma}(\pi(x))), \Phi_g(x)).$$

Therefore, since the action $\widehat{\mu}$ is free, we deduce that

$$\Sigma^2(g) - \Sigma^1(g) = \widetilde{(T^*\phi)}_{g^{-1}} \circ \widetilde{\sigma} \circ \phi_g - \widetilde{\sigma} = \delta_\phi(-\widetilde{\sigma})(g),$$

that is, $[\Sigma^1] = [\Sigma^2]$.

Conversely, if $[\Sigma^1] = [\Sigma^2]$, then there exists a Lagrangian section $\widetilde{\sigma}$ of $\widetilde{\pi}_Q$ such that

$$\Sigma^1(g) - \Sigma^2(g) = \delta_\phi(\widetilde{\sigma})(g) = \widetilde{\sigma} - \widetilde{(T^*\phi)}_{g^{-1}} \circ \widetilde{\sigma} \circ \phi_g.$$

Thus, the map $\widehat{F} : M \to M$ given by

$$\widehat{F}(x) = \widehat{\mu}(\widetilde{\sigma}(\pi(x)), x), \text{ for } x \in M,$$

satisfies the conditions of the theorem. Note that

$$\widehat{F}^{-1}(y) = \widehat{\mu}(-\widetilde{\sigma}(\pi(y)), y), \text{ with } y \in M.$$

In the case of the symplectic reference associated to a complete G-Lagrangian fibration $(M, Q, \pi, \omega, \phi, \Phi)$ we have

Corollary 1 *Let $(T^*Q/\Lambda, Q, \widetilde{\pi}_Q, \widetilde{\omega}_Q, \phi, \widetilde{T^*\phi})$ be the G-symplectic reference of a complete G-Lagrangian fibration $(M, Q, \pi, \omega, \phi, \Phi)$. Then:*

1. *Every symplectic action $\Phi : G \times T^*Q/\Lambda \to T^*Q/\Lambda$ which projects on ϕ is given by*
$$\Phi_g = \widetilde{(T^*\phi)}_g \circ t_{\Sigma(g)}$$
where $\Sigma(g) : Q \to T^*Q/\Lambda$ is a section of $\widetilde{\pi}_Q : T^*Q/\Lambda \to Q$ and $t_{\Sigma(g)} : T^*Q/\Lambda \to T^*Q/\Lambda$ is the translation $t_{\Sigma_g}([\gamma_q]) = [\gamma_q] + \Sigma(g)(q)$.
2. *If $\Sigma : G \to \mathrm{Sect}(T^*Q/\Lambda)$ is a map then $\widetilde{\Phi}^{\Sigma}_g = \widetilde{(T^*\phi)}_g \circ t_{\Sigma(g)}$ defines an action on T^*Q/Λ if and only if the map Σ is a one-cocycle in the cohomology complex $(C^\bullet((G, \mathrm{Sect}(T^*Q/\Lambda)), \delta_\phi)$.*
3. *$\widetilde{\Phi}^{\Sigma}_g$ defines a symplectic action if and only if the map Σ is a one-cocycle in the cohomology complex $(C^\bullet((G, \mathrm{Sect}_L(T^*Q/\Lambda)), \delta_\phi)$.*
4. *Consider $\Sigma^1, \Sigma^2 : G \to \mathrm{Sect}_L(T^*Q/\Lambda)$ two one-cocycles in the cohomology complex $(C^\bullet(G, \mathrm{Sect}_L(T^*Q/\Lambda)), \delta_\phi)$, and $\widetilde{\Phi}^{\Sigma^1}$ and $\widetilde{\Phi}^{\Sigma^2}$ their corresponding symplectic actions on $(T^*Q/\Lambda, \widetilde{\omega}_Q)$. Then, there exists a symplectomorphism $\widetilde{F} : T^*Q/\Lambda \to T^*Q/\Lambda$ such that*
$$\begin{array}{l} \widetilde{\pi}_Q \circ \widetilde{F} = \widetilde{\pi}_Q \text{ and} \\ \widetilde{F} \circ \widetilde{\Phi}^{\Sigma^1}_g = \widetilde{\Phi}^{\Sigma^2}_g \circ \widetilde{F}, \text{ for all } g \in G \end{array}$$
if and only if $[\Sigma^1] = [\Sigma^2] \in H^1(G, \phi, \mathrm{Sect}_L(T^*Q/\Lambda))$.

Finally, another application of our results is related with magnetic cotangent bundles.

Indeed, suppose that β is a closed 2-form on Q and consider the symplectic structure on T^*Q given by $\omega_{Q,\beta} := \omega_Q + \pi_Q^*\beta$. Then, it is easy to prove that

$\pi_Q : (T^*Q, \omega_{Q,\beta}) \to Q$ is a complete Lagrangian fibration. Moreover, in this case, the Lagrangian submanifold Λ of T^*Q is just the zero section and, thus, the symplectic reference of $\pi_Q : (T^*Q, \omega_{Q,\beta}) \to Q$ is the standard canonical projection $\pi_Q : (T^*Q, \omega_Q) \to Q$.

On the other hand, if $\phi : G \times Q \to Q$ is an action of G on Q and $g \in G$ then

$$(T^*\phi)_g^*(\omega_{Q,\beta}) = \omega_Q + \pi_Q^*(\phi_g^*\beta).$$

So, if β is G-invariant, we deduce that the cotangent lift of ϕ is a symplectic action for the total space of the complete Lagrangian fibration

$$\pi_{Q,\beta} : (T^*Q, \omega_{Q,\beta}) \to Q.$$

Using the previous facts, Proposition 5 and Theorem 4, we deduce the following result.

Corollary 2 *Let $\phi : G \times Q \to Q$ be an action of the Lie group G on the manifold Q and β be a closed 2-form which is G-invariant.*

1. *If $\Phi : G \times T^*Q \to T^*Q$ is a symplectic action of a Lie group G on $(T^*Q, \omega_Q + \pi_Q^*\beta)$ whose projection on Q is the action $\phi : G \times Q \to Q$, then there exists a differentiable map $A : G \times Q \to T^*Q$ such that*
   (a) *A is fibered on Q, i.e. $\pi_Q \circ A = pr_2$,*
   (b) *For each $g \in G$, the 1-form A_g on Q is closed.*
   (c) *The action Φ is given by*
   $$\Phi_g = (T^*\phi)_g \circ t_{A(g)}, \text{ for all } g \in G.$$
2. *If $A : G \times Q \to T^*Q$ is a smooth map and $\Phi^A : G \times T^*Q \to T^*Q$ is given by $\Phi_g^A = (T^*\phi)_g \circ t_{A(g)}$ then Φ^A is an action if and only if A is a one-cocycle in the cohomology complex $(C^\bullet(G, \Omega^1(Q)), \delta_\phi)$.*
3. *Φ^A is also symplectic if and only if $A(g)$ is a closed 1-form on Q, for all $g \in G$.*
4. *If $A, B : G \to \Omega_c^1(Q)$ are two one-cocycles in the cohomology complex $(C^\bullet(G, \Omega_c^1(Q)), \delta_\phi)$, and Φ^A and Φ^B their respective affine symplectic actions on $(T^*Q, \omega_Q + \pi^*\beta)$, then exists a symplectomorphism $F : T^*Q \to T^*Q$ such that*
   $$\pi_Q \circ F = \pi_Q \text{ and}$$
   $$F \circ \Phi_g^A = \Phi_g^B \circ F, \text{ for all } g \in G$$
   if and only if $[A] = [B] \in H^1(G, \phi, \Omega_c^1(Q))$.

Acknowledgements The authors have been partially supported by the Ministerio de Ciencia e Innovación (Spain) projects MTM2015-64166-C2-1-P and PGC2018-098265-B-C32. We also would like to thank D. Rodríguez and M. Teixidó for their useful comments.

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Chapter 18
Some Properties of Multisymplectic Manifolds

Narciso Román-Roy

Abstract This lecture is devoted to review some of the main properties of multisymplectic geometry. In particular, after reminding the standard definition of multisymplectic manifold, we introduce its characteristic submanifolds, the canonical models, and other relevant kinds of multisymplectic manifolds, such as those where the existence of Darboux-type coordinates is assured. The Hamiltonian structures that can be defined in these manifolds are also studied, as well as other important properties, such as their invariant forms and the characterization by automorphisms.

18.1 Introduction

Although there are several geometrical models for describing classical field theories, namely, *polysymplectic*, *k-symplectic* and *k-cosymplectic manifolds* [12, 17, 22, 28, 29]; *multisymplectic manifolds* are the most general and complete tool for describing geometrically (covariant) first and higher-order field theories (see, for instance, [1, 4, 8, 14, 16, 18, 20, 23, 27, 30, 32] and the references quoted on them). All of these kinds of manifolds are generalizations of the concept of *symplectic manifold*, which is used to describe geometrically mechanical (autonomous) systems.

This talk is devoted to review some of the main properties of multisymplectic geometry and is mainly based on the results presented in [5, 6, 9, 13, 21]. In particular we discuss the following topics: the basic definition of *multisymplectic manifold* (in Sect. 18.2) and the *Hamiltonian structures* associated to a multisymplectic form (Sect. 18.3), the characteristic submanifolds of multisymplectic manifolds (Sect. 18.4), the canonical models and the existence of Darboux-type coordinates (Sect. 18.5), other kinds of relevant multisymplectic manifolds (Sect. 18.6) and, finally, some interesting theorems of invariance and characterization by automorphisms (Sect. 18.7).

N. Román-Roy (✉)
Department of Mathematics, Ed. C-3, Campus Norte UPC, C/ Jordi Girona 1,
08034 Barcelona, Spain
e-mail: narciso.roman@upc.edu

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_18

All the manifolds are real, second countable and C^∞. The maps and the structures are C^∞. Sum over repeated indices is understood.

18.2 Multisymplectic Manifolds

(See [5, 6, 13] for more details).

Definition 1 Let M be a differentiable manifold, with $\dim M = n$, and $\Omega \in \Omega^k(M)$ ($\Omega^k(M)$ denotes the set of differentiable k-forms in M), with $k \leq n$.

- The form Ω is 1-nondegenerate if, for every $p \in M$ and $X_p \in \mathrm{T}_pM$,

$$i(X_p)\Omega_p = 0 \iff X_p = 0\,.$$

- The form Ω is a multisymplectic form if it is closed and 1-nondegenerate.
- A multisymplectic manifold of degree k is a couple (M, Ω), where $\Omega \in \Omega^k(M)$ is a multisymplectic form.

If Ω is only closed then it is called a pre-multisymplectic form.
If Ω is only 1-nondegenerate then it is an almost-multisymplectic form.

If $\dim M \geq 2$, then a multisymplectic k-form must have degree $k \geq 2$.

The property of 1-nondegeneracy can be characterized equivalently as follows: a differentiable k-form Ω is 1-nondegenerate if, and only if, the vector bundle morphism

$$\begin{aligned} \Omega^\flat \colon \mathrm{T}M &\to \Lambda^{k-1}\mathrm{T}^*M \\ X_p &\mapsto i(X_p)\Omega_p \end{aligned}$$

and thus the corresponding morphism of $C^\infty(M)$-modules

$$\begin{aligned} \Omega^\flat \colon \mathfrak{X}(N) &\to \Omega^{k-1}(N) \\ X &\mapsto i(X)\Omega \end{aligned}$$

are injective.

Some examples of multisymplectic manifolds are the following: Multisymplectic manifolds of degree 2 are just *symplectic manifolds*. Multisymplectic manifolds of degree n are *orientable manifolds* and the multisymplectic forms are *volume forms*. *Bundles of k-forms* (*k-multicotangent bundles*) endowed with their *canonical $(k+1)$-forms* are multisymplectic manifolds of degree $k+1$. *Jet bundles* (over m-dimensional manifolds) endowed with the *Poincaré-Cartan $(m+1)$-forms* associated with (singular)*Lagrangian densities* are (pre)multisymplectic manifolds of degree $m+1$.

18.3 Hamiltonian Structures in Multisymplectic Manifolds

(See [5, 6, 13] for more details).

Definition 2 A m-vector field (or a multivector field of degree m) in a manifold M (with $m \leq n = \dim M$) is any section of the bundle $\Lambda^m(\mathrm{T}M) \to M$ (that is, a contravariant, skewsymmetric tensor field of degree m in M). The set of m-vector fields in M is denoted by $\mathfrak{X}^m(M)$.

The local description of multivector fields of degree m is the following: for every $p \in M$, there are a neighbourhood $U_p \subset M$ and local vector fields $X_1, \ldots, X_r \in \mathfrak{X}(U_p)$, with $m \leq r \leq \dim M$, such that

$$\mathbf{X}|_{U_p} = \sum_{1 \leq i_1 < \ldots < i_m \leq r} f^{i_1 \ldots i_m} X_{i_1} \wedge \ldots \wedge X_{i_m} \; ; \quad \text{with } f^{i_1 \ldots i_m} \in \mathrm{C}^\infty(U_p) \; . \tag{18.1}$$

Definition 3 Let $\mathbf{X} \in \mathfrak{X}^m(M)$ be a multivector field.
$\mathbf{X}$ is homogeneous (or decomposable) if there are $X_1, \ldots, X_m \in \mathfrak{X}(M)$ such that $\mathbf{X} = X_1 \wedge \ldots \wedge X_m$.
$\mathbf{X}$ is locally homogeneous (decomposable) if, for every $p \in M$, there exist $U_p \subset M$ and $X_1, \ldots, X_m \in \mathfrak{X}(U_p)$ such that $\mathbf{X}|_{U_p} = X_1 \wedge \ldots \wedge X_m$.

Remark 1 Locally decomposable m-multivector fields $\mathbf{X} \in \mathfrak{X}^m(M)$ are locally associated with m-dimensional distributions $D \subset \mathrm{T}M$.

Every multivector field $\mathbf{X} \in \mathfrak{X}^m(M)$ defines a *contraction* with differential forms $\Omega \in \Omega^k(M)$, which is the natural contraction between tensor fields. In particular, if $\mathbf{X}$ is expressed as in (18.1), we have

$$\begin{aligned} i(\mathbf{X})\Omega|_{U_p} &= \sum_{1 \leq i_1 < \ldots < i_m \leq r} f^{i_1 \ldots i_m} i(X_1 \wedge \ldots \wedge X_m)\Omega \\ &= \sum_{1 \leq i_1 < \ldots < i_m \leq r} f^{i_1 \ldots i_m} i(X_1) \ldots i(X_m)\Omega \; . \end{aligned}$$

Then, the k-form Ω is said to be *j-nondegenerate* (for $1 \leq j \leq k-1$) if, for every $p \in E$ and $\mathbf{Y} \in \mathfrak{X}^j(M)$, we have that $i(\mathbf{Y}_p)\Omega_p = 0$ if, and only if, $\mathbf{Y}_p = 0$.

Then, for every form $\Omega \in \Omega^k(M)$ ($k \geq m$) we have the morphisms

$$\begin{array}{ccccc} \Omega^\flat : \Lambda^m(\mathrm{T}M) & \longrightarrow & \Lambda^{k-m}(\mathrm{T}^*M) & ; & \Omega^\flat : \mathfrak{X}^m(M) & \longrightarrow & \Omega^{k-m}(M) \\ \mathbf{X}_p & \mapsto & i(\mathbf{X}_p)\Omega_p & & \mathbf{X} & \mapsto & i(\mathbf{X})\Omega \end{array} \; .$$

In addition, if $\mathbf{X} \in \mathfrak{X}^m(M)$, the *Lie derivative* of $\Omega \in \Omega^k(M)$ is

$$\mathrm{L}(\mathbf{X})\Omega := [\mathrm{d}, i(\mathbf{X})]\Omega = \mathrm{d}i(\mathbf{X})\Omega - (-1)^m i(\mathbf{X})\mathrm{d}\Omega \; .$$

Definition 4 Let (M, Ω) be a multisymplectic manifold of degree k. A diffeomorphism $\varphi: M \to M$ is a multisymplectomorphism if $\varphi^*\Omega = \Omega$.

Definition 5 Let (M, Ω) be a multisymplectic manifold of degree k.

1. A vector field $X \in \mathfrak{X}(M)$ is a locally Hamiltonian vector field if its flow consists of multisymplectic diffeomorphisms. It is equivalent to demand that $\mathrm{L}(X)\Omega = 0$, or equivalently, $i(X)\Omega \in \Omega^{k-1}(M)$ is a closed form.
2. A multivector field $\mathbf{X} \in \mathfrak{X}^m(M)$ $(m < k)$ is a locally Hamiltonian multivector field if $\mathrm{L}(\mathbf{X})\Omega = 0$ or, what is equivalent, $i(\mathbf{X})\Omega \in \Omega^{k-m}(M)$ is a closed form. Then, for every $p \in M$, exist $U \subset M$ and $\zeta \in \Omega^{k-m-1}(U)$ such that $i(\mathbf{X})\Omega = \mathrm{d}\zeta$ (on U).
   In this case $\zeta \in \Omega^{k-m-1}(U)$ is said to be a locally Hamiltonian form for $\mathbf{X}$.
3. $\mathbf{X} \in \mathfrak{X}^m(M)$ is a Hamiltonian multivector field if $i(\mathbf{X})\Omega \in \Omega^{k-m}(M)$ is an exact form; that is, there exists $\zeta \in \Omega^{k-m-1}(M)$ such that $i(\mathbf{X})\Omega = \mathrm{d}\zeta$.
   In this case $\zeta \in \Omega^{k-m-1}(M)$ is said to be a Hamiltonian form for $\mathbf{X}$.

18.4 Characteristic Submanifolds of Multisymplectic Manifolds

(See [6, 9] for more details and proofs).

Definition 6 Let (M, Ω) be a multisymplectic manifold of degree k, and $\mathcal{W}$ a distribution in M. $\forall p \in M$ and $1 \leq r \leq k-1$, the r-orthogonal multisymplectic vector space at p is

$$\mathcal{W}_p^{\perp,r} = \{v \in \mathrm{T}_pM \mid i(v \wedge w_1 \wedge \ldots \wedge w_r)\Omega_p = 0,\ \forall w_1, \ldots, w_r \in \mathcal{W}_p\}\ ,$$

the r-orthogonal multisymplectic complement of $\mathcal{W}$ is the distribution $\mathcal{W}^{\perp,r} := \cup_{p\in M}\mathcal{W}_p^{\perp,r}$.

1. $\mathcal{W}$ is an r-coisotropic distribution if $\mathcal{W}^{\perp,r} \subset \mathcal{W}$.
2. $\mathcal{W}$ is an r-isotropic distribution if $\mathcal{W} \subset \mathcal{W}^{\perp,r}$.
3. $\mathcal{W}$ is an r-Lagrangian distribution if $\mathcal{W} = \mathcal{W}^{\perp,r}$.
4. $\mathcal{W}$ is a multisymplectic distribution if $\mathcal{W} \cap \mathcal{W}^{\perp,k-1} = \{0\}$.

Remark 2 For every distribution $\mathcal{W}$, we have that $\mathcal{W}^{\perp,r} \subset \mathcal{W}^{\perp,r+1}$. As a consequence, every r-isotropic distribution is $(r+1)$-isotropic, and every r-coisotropic distribution is $(r-1)$-coisotropic.

As a particular situation, if we have a submanifold N of multisymplectic manifold M, we can take as distribution in $\mathrm{T}M$ the tangent bundle $\mathrm{T}N$ and this allows us to establish a classification of these submanifolds as follows:

Definition 7 Let (M, Ω) be a multisymplectic manifold of degree k, and N a submanifold of M. If $0 \leq r \leq k-1$, then:

1. N is an r-coisotropic submanifold of M if $\mathrm{T}N^{\perp,r} \subset \mathrm{T}N$.
2. N is an r-isotropic submanifold of M if $\mathrm{T}N \subset \mathrm{T}N^{\perp,r}$.
3. N is an r-Lagrangian submanifold of M if $\mathrm{T}N = \mathrm{T}N^{\perp,r}$.
4. N is a multisymplectic submanifold of M if $\mathrm{T}N \cap \mathrm{T}N^{\perp,k-1} = \{0\}$.

And, in particular we have:

Proposition 1 *A submanifold N of M is r-Lagrangian if, and only if, it is r-isotropic and maximal.*

18.5 Canonical Models for Multisymplectic Manifolds. Darboux-Type Coordinates

(See [9] for more details).

In the same way as the tangent bundle of a manifold is the canonical model for symplectic manifolds, the canonical models of multisymplectic manifolds are the *bundles of forms*. These canonical models are constructed as follows:

- If Q is a manifold, the bundle $\rho\colon \Lambda^k(\mathrm{T}^*Q) \to Q$ is the *bundle of k-forms* in Q. The *tautological form* (or *canonical form*) $\Theta_Q \in \Omega^k(\Lambda^k(\mathrm{T}^*Q))$ is defined as follows: if $\alpha \in \Lambda^k(\mathrm{T}^*Q)$, and $V_1, \ldots, V_k \in \mathrm{T}_\alpha(\Lambda^k(\mathrm{T}^*Q))$, then

$$\Theta_{Q_\alpha}(V_1, \ldots, V_k) = i(\rho_* V_k \wedge \ldots \wedge \rho_* V_1)\alpha \ .$$

  We have that, $\Omega_Q = \mathrm{d}\Theta_Q \in \Omega^{k+1}(\Lambda^k(\mathrm{T}^*Q))$ is a 1-nondegenerate form and then $(\Lambda^k(\mathrm{T}^*Q), \Omega_Q)$ is a multisymplectic manifold of degree $k+1$.
  If $(x^i, p_{i_1\ldots i_k})$ is a system of *natural coordinates* in $U \subset \Lambda^k(\mathrm{T}^*Q)$, then the local expressions of these canonical forms are

$$\Theta_Q \mid_U = p_{i_1\ldots i_k}\mathrm{d}x^{i_1} \wedge \ldots \wedge \mathrm{d}x^{i_k} \quad , \quad \Omega_Q \mid_U = \mathrm{d}p_{i_1\ldots i_k} \wedge \mathrm{d}x^{i_1} \wedge \ldots \wedge \mathrm{d}x^{i_k} \ .$$

  These are called *Darboux coordinates* in $\Lambda^k(\mathrm{T}^*Q)$.
- If $\pi : Q \to E$ is a fibration, let $\rho_r\colon \Lambda^k_r(\mathrm{T}^*Q) \to Q$ be the subbundle of $\Lambda^k(\mathrm{T}^*Q)$ made of the r-horizontal k-forms in Q with respect to the projection π (that is, the k-forms in Q vanishing when applied to r π-vertical vector fields in Q).
  Let $\Theta^r_Q \in \Omega^k(\Lambda^k_r(\mathrm{T}^*Q))$ be the pull-back of Θ_Q to $\Lambda^k_r(\mathrm{T}^*Q)$. This is the tautological k-form in $\Lambda^k_r(\mathrm{T}^*Q)$, and then, if we construct $\Omega^r_Q = \mathrm{d}\Theta^r_Q \in \Omega^{k+1}(\Lambda^k_r(\mathrm{T}^*Q))$, we have that $(\Lambda^k_r(\mathrm{T}^*Q), \Omega^r_Q)$ is also a multisymplectic manifold of degree $k+1$.
  In the same way, there are also charts of Darboux coordinates in $\Lambda^k_r(\mathrm{T}^*Q)$ on which these canonical forms have a local expressions similar to the above ones.

Nevertheless, unlike symplectic manifolds, multisymplectic manifolds (M, Ω) in general are not (locally) diffeomorphic to their canonical models, and additional

properties are needed in order to have a Darboux theorem which assures the existence of Darboux-type coordinates [26]. In particular:

Definition 8 A special multisymplectic manifold is a multisymplectic manifold (M, Ω) of degree k such that:

1. $\Omega = \mathrm{d}\Theta$, for some $\Theta \in \Omega^{k-1}(M)$.
2. There is a diffeomorphism $\phi\colon M \to \Lambda^{k-1}(\mathrm{T}^*Q)$, $\dim Q = n \geq k-1$, (or $\phi\colon M \to \Lambda^{k-1}_r(\mathrm{T}^*Q)$), and a fibration $\pi : M \to Q$ such that $\rho \circ \phi = \pi$ (resp. $\rho_r \circ \phi = \pi$), and $\phi^*\Theta_Q = \Theta$ (resp. $\phi^*\Theta^r_Q = \Theta$).
(It is said that (M, Ω) is multisymplectomorphic to a bundle of forms).

In order to have multisymplectic manifolds which locally behave as the canonical models, it is necessary to endow them with additional structures; in particular, a 1-isotropic distribution $\mathcal{W}$ satisfying some dimensionality conditions, and a "generalized distribution" ε defined on the space of leaves determined by $\mathcal{W}$. In fact, the existence of distributions satisfying certain properties is a necessary condition in order to establish Darboux-type theorems for different kinds of geometrical structures (presymplectic, cosymplectic, k-symplectic, and k-cosymplectic) [2, 7, 10, 11]. Thus:

Definition 9 Let (M, Ω) be a multisymplectic manifold of degree k, and $\mathcal{W}$ a regular 1-isotropic involutive distribution in (M, Ω).

1. A multisymplectic manifold of type $(k, 0)$ is a triple $(M, \Omega, \mathcal{W})$ such that, for every $p \in M$, we have that:
   a. $\dim \mathcal{W}(p) = \dim \Lambda^{k-1}(\mathrm{T}_pM/\mathcal{W}(p))^*$.
   b. $\dim (\mathrm{T}_pM/\mathcal{W}(p)) > k-1$.
2. A multisymplectic manifold of type (k, r) $(1 \leq r \leq k-1)$ is a quadruple $(M, \Omega, \mathcal{W}, \mathcal{E})$, where $\mathcal{E}$ is a "generalized distribution" on M (this means that, for every $p \in M$, $\mathcal{E}(p)$ is a vector subspace of $\mathrm{T}_pM/\mathcal{W}(p)$) and, denoting by $\pi_p\colon \mathrm{T}_pM \to \mathrm{T}_pM/\mathcal{W}(p)$ the canonical projection, we have that:
   a. $i(v_1 \wedge \ldots \wedge v_r)\Omega_p = 0$, for every $v_i \in \mathrm{T}_pM$ such that $\pi_p(v_i) \in \mathcal{E}(p)$ $(i = 1, \ldots, r)$.
   b. $\dim \mathcal{W}(p) = \dim \Lambda^{k-1}_r(\mathrm{T}_pM/\mathcal{W}(p))^*$, where the horizontal forms are considered with respect to the subspace $\mathcal{E}(p)$.
   c. $\dim (\mathrm{T}_pM/\mathcal{W}(p)) > k-1$.

And the fundamental result is the following:

Proposition 2 *Every multisymplectic manifold (M, Ω) of type $(k, 0)$ (resp. of type (k, r)) is locally multisymplectomorphic to a bundle of $(k-1)$-forms $\Lambda^{k-1}(\mathrm{T}^*Q)$ (resp. $\Lambda^{k-1}_r(\mathrm{T}^*Q)$), for some manifold Q; that is, to a canonical multisymplectic manifold.*

Therefore, there is a local chart of Darboux coordinates *around every point $p \in M$.*

Proof The proof of this Theorem is very long and can be found in [9] (where, in particular, the relation with the canonical models is shown). □

Then we define:

Definition 10 Multisymplectic manifolds which are locally multisymplectomorphic to bundles of forms are called locally special multisymplectic manifolds.

Of course, every special multisymplectic manifold is a locally special multisymplectic manifold and hence has charts of *Darboux coordinates* at every point.

As an interesting example, if $\pi : E \to M$ is a fiber bundle (where M is an m-dimensional oriented manifold), $J^1\pi$ is the corresponding first-order jet bundle, and $\mathcal{L}$ is a first-order hyperregular Lagrangian density, then the Poincaré-Cartan form $\Omega_{\mathcal{L}} \in \Omega^{m+1}(J^1\pi)$ is a multisymplectic form and $(J^1\pi, \Omega_{\mathcal{L}})$ is a special multisymplectic manifold [4, 15, 30].

18.6 Other Kinds of Multisymplectic Manifolds

(See [13] for more details).

It is a well-known property of symplectic manifolds that the set of local Hamiltonian vector fields span locally the tangent bundle of the manifold and, hence, the action of the group of multisymplectic diffeomorphisms on M is transitive (in fact, these properties are a consequence of the existence of Darboux coordinates). Nevertheless, in general, these properties do not hold for multisymplectic manifolds and so locally Hamiltonian vector fields in a multisymplectic manifold (M, Ω) do not span the tangent bundle of this manifold, and the group of multisymplectic diffeomorphisms does not act transitively on M. In order to achieve this we need to introduce additional conditions. Hence, we define:

Definition 11 Let M be a differentiable manifold, $p \in M$ and a compact set K with $p \in \overset{\circ}{K}$. A local Liouville or local Euler-like vector field at p with respect to K is a vector field $\Delta^p \in \mathfrak{X}(M)$ such that:

1. $\operatorname{supp} \Delta^p := \overline{\{x \in M \mid \Delta^p(x) \neq 0\}} \subset K$,
2. there exists a diffeomorphism $\varphi\colon \overbrace{\operatorname{supp} \Delta^p}^{\circ} \to \mathbb{R}^n$ such that $\varphi_* \Delta^p = \Delta$, where $\Delta = x^i \dfrac{\partial}{\partial x^i}$ is the standard Liouville or dilation vector field in $\mathbb{R}^n$.

Definition 12 A form $\Omega \in \Omega^k(M)$ is said to be locally homogeneous at $p \in M$ if, for every open set $U \subset M$ containing p, there exists a local Euler-like vector field Δ^p at p with respect to a compact set $K \subset U$ such that

$$\mathrm{L}(\Delta^p)\Omega = f\,\Omega\,; \quad f \in \mathrm{C}^\infty(U)\,.$$

Ω is locally homogeneous if it is locally homogeneous for all $p \in M$.

A locally homogeneous manifold is a couple (M, Ω), where M is a manifold and $\Omega \in \Omega^k(M)$ is locally homogeneous.

Therefore we have that:

Proposition 3 *Let (M, Ω) be a locally homogeneous multisymplectic manifold. Then the family of locally Hamiltonian vector fields span locally the tangent bundle of M; that is, $\forall\, p \in M$, $\mathrm{T}_pM = \mathrm{span}\{X_p \mid X \in \mathfrak{X}(M)\ ,\ \mathrm{L}(X)\Omega = 0\}$.*

Proof (Outline of the proof): The proof is very technical (see [13] for all the details). First, the existence of local Euler-like vector fields and their properties allows us to prove a previous result known as the *localization Lemma* which states that, if X is a locally Hamiltonian vector field, and $x_0 \in M$, then for each open set $U \ni x_0$, there exists an open neighbourhood V of x_0 such that $V \subset \bar{V} \subset U$, with $\bar{V}$ compact, and a locally Hamiltonian vector field X' such that X' coincides with X in V and vanishes identically outside of U. Then, the proof of this Proposition follows from the aplication of this Lemma and using again Euler-like vector fields. □

Theorem 1 *The group of multisymplectic diffeomorphisms $G(M, \Omega)$ of a locally homogeneous multisymplectic manifold (M, Ω) acts transitively on M.*

Proof (Outline of the proof [13]): The proof is based on the application of Proposition 3 and the above mentioned localization Lemma. □

Remark 3 Locally special multisymplectic manifolds have local Euler-like vector fields; in particular, the local vector fields $\left\{ x^i \dfrac{\partial}{\partial x^i} + p_{i_1 \dots i_k} \dfrac{\partial}{\partial p_{i_1 \dots i_k}} \right\}$. Then, the corresponding multisymplectic forms are locally homogeneous.

As a consequence, if (M, Ω) is a locally special multisymplectic manifold, then the family of locally Hamiltonian vector fields span locally the tangent bundle of M and the group of multisymplectic diffeomorphisms acts transitivelly on M. In fact, the local vector fields $\left\{ \dfrac{\partial}{\partial x^i}, \dfrac{\partial}{\partial p_{i_1 \dots i_k}} \right\}$ are locally Hamiltonian.

18.7 Invariance Theorems

(See [13, 21] for more details).

As final remarks, in this Section we generalize some classical theorems of symplectic geometry in the field of multisymplectic manifolds.

The first one is a partial generalization of *Lee Hwa Chung's Theorem* for symplectic manifolds, which characterizes all the differential forms which are invariant under infinitesimal symplectomorphisms [19, 24, 25]:

Theorem 2 *Let (M, Ω) be a locally homogeneous multisymplectic manifold of degree k and $\alpha \in \Omega^p(M)$, with $p = k - 1, k$, such that:*

(i) The form α is invariant by the set of locally Hamiltonian $(k-1)$-vector fields; that is, $\mathrm{L}(\mathbf{X})\alpha = 0$, *for every* $\mathbf{X} \in \mathfrak{X}^{k-1}_{lh}(M)$.
(ii) The form α is invariant by the set of locally Hamiltonian vector fields; that is, $\mathrm{L}(Z)\alpha = 0$, *for every* $Z \in \mathfrak{X}_{lh}(M)$.

Therefore:

1. *If $p = k$ then $\alpha = c\,\Omega$, with $c \in \mathbb{R}$.*
2. *If $p = k-1$ then $\alpha = 0$.*

Proof (Outline of the proof [13]): It is an adaptation of the proofs given in [19, 25] for presymplectic and symplectic manifolds. From the hypothesis of the Theorem and bearing in mind the properties stated in Sect. 18.3, it can be proved that, for every $X, Y \in \mathfrak{X}^{k-1}_{lh}(M)$, the following relation holds: $i(X)\Omega \wedge i(Y)\alpha + i(Y)\Omega \wedge i(X)\alpha = 0$; and taking $X \in \ker^{k-1}\Omega$, from here you get to $i(X)\alpha = 0$. Then it is proved that, if $p = k-1$ then $\alpha = 0$; but, if $p = k$, then there exists a unique $\alpha' \in \mathrm{C}^\infty(M)$ such that $i(X)\alpha = \alpha' i(X)\Omega$, for every $X \in \mathfrak{X}^{k-1}_{lh}(M)$. Therefore, using some local properties of the locally Hamiltonian $(k-1)$-multivector fields, it is concluded that α' is constant and the final conclusion follows straightforwardly from the last results and Proposition 3. □

The second one is a generalization of some *Theorems of Banyaga* for symplectic and other orientable manifolds [3]:

Theorem 3 *Let (M_i, Ω_i), $i = 1, 2$, be local homogeneous multisymplectic manifolds of degree k and $G(M_i, \Omega_i)$ their groups of multisymplectic automorphisms. Let $\Phi\colon G(M_1, \Omega_1) \to G(M_2, \Omega_2)$ be a group isomorphism (which is a homeomorphism when $G(M_i, \Omega_i)$ are endowed with the point-open topology). Then, there exists a diffeomorphism $\varphi\colon M_1 \to M_2$, such that:*

1. *$\Phi(\psi) = \varphi \circ \psi \circ \varphi^{-1}$, for every $\psi \in G(M_1, \Omega_1)$.*
2. *The map φ_* maps locally Hamiltonian vector fields of (M_1, Ω_1) into locally Hamiltonian vector fields of (M_2, Ω_2).*
3. *In addition, if φ_* maps locally Hamiltonian multivector fields of (M_1, Ω_1) into locally Hamiltonian multivector fields of (M_2, Ω_2), then there is a constant c such that $\varphi^*\Omega_2 = c\,\Omega_1$.*

Proof (Outline of the proof [13]): By Theorem 1, $G(M_i, \Omega_i)$ acts transitively on M_i and, by the main theorem in [33], there exists a bijective map $\varphi\colon M_1 \to M_2$ such that $\Phi(\psi) = \varphi \circ \psi \circ \varphi^{-1}$. Then it is proved that φ is a homeomorphism and, adapting the proof in [3] to our setting, that it is also a smooth diffeomorphism. Therefore, as a consequence of this proof, we conclude that φ_* maps locally Hamiltonian vector fields into locally Hamiltonian vector fields. Finally, assuming the hypothesis of the third item, using Theorem 2 we have that $\varphi^*\Omega_2 = c\,\Omega_1$. □

18.8 Conclusions and Discussion

Some of the main properties and characteristics of multisymplectic manifolds have been reviewed in this dissertation. Although most of them are generalizations of other well-known results for symplectic geometry, in the multisymplectic case, they are more elaborated and richer than for symplectic manifolds, in general; and it is for this reason that this is a topic of active research [31].

In particular, other interesting properties of multisymplectic manifolds which have not been analyzed here are, for instance: the *graded Lie algebra structure* of the sets of *Hamiltonian forms* and *Hamiltonian multivector fields* [5, 13], *polarized multisymplectic manifold* and its general structure theorem [6], as well as other properties and relevance of r-coisotropic, r-isotropic and, especially, of r-Lagrangian distributions and submanifols [6, 9], and the characterizations of multisymplectic transformations [13].

Acknowledgements I acknowledge the financial support of the *Ministerio de Ciencia e Innovación* (Spain), projects MTM2014–54855–P and MTM2015-69124–REDT, and of *Generalitat de Catalunya*, project 2017–SGR–932.

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Chapter 19
A Simple Model of Double Dynamics on Lie Groups

Patrizia Vitale

Abstract We study the dynamics of the rigid rotator on the group manifold of $SU(2)$ as an instance of dynamics on Lie groups together with a dual model whose carrier space is the Borel group $SB(2, \mathbb{C})$, the Lie Poisson dual of $SU(2)$. We thus introduce a parent action on the Drinfel'd double of the above mentioned groups, which describes the dynamics of a system with twice as many degrees of freedom as the two starting partners. Through a gauging procedure of its global symmetries both the rigid rotor and the dual model are recovered.

19.1 Introduction

This paper is based on a lecture given at the conference in honour of Alberto Ibort,"Classical and Quantum Physics: Geometry, Dynamics and Control" at ICMAT, Madrid, in March 2018, and it is aimed at discussing within a simple example of dynamics over Lie groups, the isotropic rigid rotator (IRR), the interplay between concepts such as non-Abelian and Poisson-Lie T-duality [1–3], Generalized and Doubled Geometry [4–7], Double Field Theory (DFT) [8], in the mathematical framework of Poisson-Lie groups and Drinfel'd doubles [9, 10]. The main goal being here to convey the general philosophy, many technical details and in deep calculations are left aside and we refer to [11] for an extended presentation of the results. A generalization to field theory can be found in [12].

The cotangent space of a d dimensional Lie group, G, $T^*G \sim G \times \mathbb{R}^d$, while providing the carrier space for the Hamiltonian dynamics of many systems of physical relevance, possesses a very interesting structure from the mathematical point of view, it being itself a Lie group, the semi-direct product of the Lie group G with the dual of its Lie algebra, the Abelian Lie algebra $\mathfrak{g}^* \sim \mathbb{R}^d$, thought of as an Abelian vector group. Free dynamics over the group manifold is described in terms of momenta,

P. Vitale (✉)
Dipartimento di Fisica "E. Pancini", Università di Napoli Federico II and INFN-Sezione di Napoli, Complesso Universitario di Monte S. Angelo Edificio 6, via Cintia, 80126 Napoli, Italy
e-mail: patrizia.vitale@na.infn.it

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_19

$I_i, i = 1, ..., d$ which are coordinate variables for the fiber $\mathfrak{g}^*$, with Hamiltonian evolution governed by Kirillov-Souriau-Konstant (KSK) Poisson brackets $\{I_i, I_j\} = c_{ij}^k I_k$ and c_{ij}^k the structure constants of the Lie algebra $\mathfrak{g}$.

The first interesting remark, although well known, is thus that, as a Lie group $\mathfrak{g}^*$ is Abelian, but the Poisson algebra of linear functions over $\mathfrak{g}^*$, is non-Abelian and isomorphic to the Lie algebra $\mathfrak{g}$. Moreover the latter can be obtained by linearizing the so-called Poisson-Lie structure over the dual group of G which shall be indicated by G^*[13].

The tangent bundle TG has the structure of a group, with its fiber which is isomorphic to the Lie algebra $\mathfrak{g}$, typically non-Abelian. Fiber coordinates, namely the generalized velocities, are components of left or right invariant vector fields $X_a = \dot{Q}^i_{(a)} \frac{\partial}{\partial Q^i}, a = 1, ..., d$ with non-trivial Lie brackets $[X_a, X_b] = c^c_{ab} X_c$.

Models which exchange tangent and cotangent bundle coordinates over Lie groups, have been widely studied in the context of field theory of sigma models and the duality which is naturally inherited from the relation between the Lie algebra and its dual, is referred to as non-Abelian, or semi-Abelian duality [1]. According to the structure which we have outlined, the dual model in such context relies on a Poisson algebra of momenta which is Abelian. The IRR system, which we are going to investigate in the paper, can be regarded as a $0 + 1$ dimensional analogue of a non-linear sigma model with target space $SU(2)$.

Once identified the cotangent space of the Lie group G with a semi-direct product of groups, the second interesting observation is that there exists a well defined procedure for deforming the semi-direct product into a fully non-Abelian group, by introducing a non-trivial Lie algebra structure over $\mathfrak{g}^*$, so that the cotangent space $G \ltimes \mathbb{R}^d$ be replaced by $D \simeq G \cdot G^*$ (the latter trivialization being only local) with G^* the Lie group obtained by $\mathfrak{g}^*$ by exponentiation. The group D is the Drinfel'd double of G. Since the role of G and G^* is symmetric, D can be dually regarded as the double of G^* and hence, as a deformation of the cotangent bundle T^*G^*.[1] Therefore a dynamical system can be defined with the latter as carrier space of the dynamics. The new algebra of momenta, being dictated by the KSK Poisson brackets $\{\tilde{I}^i, \tilde{I}^j\} = f_k^{ij} \tilde{I}^k$ (f_k^{ij} the structure constants of G^*), can be retrieved by linearizing the Poisson-Lie bracket over G [11]. Therefore, the IRR model and the latter one are dual to each other, in the sense that they are defined over partner groups in the Drinfel'd double D, with linearized Poisson-Lie brackets of momenta. This is a kind of Poisson-Lie duality, although the name has already been used in the literature in the context of sigma models [2], implying a more stringent relation, which we will comment in due time. Completely integrable systems and their relation to double Lie groups have been studied in [14].

A natural step further is to consider a parent action over the Drinfel'd double D with twice as many degrees of freedom as the two actions over G, G^* respectively. Such a doubling will generate a Double Field Theory when considering the 1+1-

[1] Notice however that, in case G is a compact group, such as $SU(2)$, its cotangent bundle is truly diffeomorphic to its Drinfel'd double, while the cotangent bundle of its dual, $SB(2\mathbb{C})$ for $SU(2)$, is only a deformation of the double.

dimensional analogue of the IRR model [12]. The generalized action encodes the global symmetries of both models and can be reduced to either of them by means of an appropriate gauging of some of the symmetries. The generalized momenta $\mathbf{P_I}$ being sections of the cotangent bundle T^*D can be described in terms of the momenta of the cotangent spaces of the dually related groups G, G^*: $\mathbf{P_I} \simeq (I_i, \tilde{I}^i)$, where the position of indices stresses the dual geometric meaning of the two. Because the cotangent fibre of one group can be identified with the tangent fiber of the other and vice-versa, the connection with Generalized Geometry is thus natural.

The latter was first introduced by Hitchin in [4]. Shortly, it consists in replacing the tangent bundle T of a manifold M with $T \oplus T^*$, a bundle with the same base space M but fibers given by the direct sum of tangent and cotangent spaces. Moreover, the Lie bracket on the sections of T, which are vector fields, is replaced by the Courant bracket which involves vector fields and one-forms. This is in turn related to Double Field Theory (DFT) [8].

DFT was introduced to realize the symmetry of the dynamics of string theory under target space duality transformations as a manifest symmetry of the string action. In order to achieve this goal, the degrees of freedom of the target space, represented by the coordinate fields $x^i(\sigma, \tau)$, $i = 1, \ldots, d$ have to be *doubled* with respect to the starting model. Therefore, in the framework of string theory, the doubling takes place in the d-dimensional target space M of the non-linear sigma model underlying the string action, by introducing new fields $\tilde{x}_i(\sigma, \tau)$, which are dual to $x^i(\sigma, \tau)$, with $i = 1, \ldots, d$. This is in perfect agreement with the approach of Generalized Geometry, by identifying $x^i, \tilde{x}_i$ with sections of a generalized bundle $E \oplus E^*$ over the world sheet of the string. Thus, it is only when the target space of the string becomes the configuration space of an *effective field theory*, that the doubling of fields is reinterpreted as a doubling of the configuration space. A formulation of the string action with manifest T-duality invariance was first proposed by [15, 16]. A corresponding doubling of the space-time degrees of freedom in the low-energy effective action first occurred in the pioneering of work of Siegel [17]. There is therefore a relation between GG and DFT which we think can be better understood within the study of the dynamics of simple models over Lie groups, where duality and doubling are naturally encoded within the notion of Drinfel'd double and dual Poisson-Lie groups [9, 10]. These geometric structures have first been introduced in the context of field theory by Klimčík and Ševera in [1], Klimčík [2] where the authors first introduced the notion of Poisson-Lie T-duality (also see [18], [19], [20]) for sigma models. DFT on group manifolds with its relation with Poisson-Lie symmetries, has been investigated in [21].

The interest for DFT is naturally not limited to string theory. The necessity of doubling the degrees of freedom occurs already in the Lagrangian/Hamiltonian formulation of dissipative dynamics [22], or, recently, within the symplectic realization of so-called twisted Poisson brackets [23–25], namely non-degenerate brackets which however violate Jacobi identity. While the latter can be related to the non-associative nature of the product emerging from the attempt of quantizing such models, the occurrence of auxiliary degrees of freedom is also a typical feature of Noncommutative

geometry.[2] For example, in order to build a noncommutative extension of Palatini-Holst theory of gravity it was pointed out in [31] that the gauge group has to be enlarged, leading to the introduction of new gravitational degrees of freedom. In particular, the tetrad degrees of freedom were doubled, thus leading to a bi-tetrad theory of gravity, generalizing a model that was previously proposed in [32].

The paper is intended to give a short account of the results contained in [11]. Therefore the structure strictly follows the former, although being less technical. In Sect. 19.2 we review the dynamics of the IRR on the group manifold of the group $SU(2)$. In Sect. 19.3 we shortly introduce the mathematical framework of Poisson-Lie groups and Drinfel'd doubles. In Sect. 19.4 we introduce a dynamical model on the dual group of $SU(2)$, the Borel group $SB(2,\mathbb{C})$ and study its dynamics. In Sect. 19.5 we propose a parent action on the Drinfel'd double, which has twice as many degrees of freedom as the two partner models. The latter are recovered by appropriately gauging the global symmetries of the former. Finally, in Sect. 19.5.1 we introduce the Hamiltonian formalism for the double model and in 19.5.2 we study in detail the full Poisson algebra. The Poisson brackets of the generalized momenta $(I_i, \tilde{I}^i)$ can be related to a first-order expansion, in some deformation parameter, of Poisson-Lie brackets on the two dual groups, thus giving rise to a kind of Poisson-Lie T-duality between the two models. The full Poisson algebra of momenta is isomorphic to the algebra of $SL(2,\mathbb{C})$, the double covering of the Lorentz group. Section 19.6 contains our conclusions.

19.2 The Isotropic Rigid Rotator

The dynamics of the three-dimensional Isotropic Rigid Rotator (IRR) can be formulated in terms of group valued dynamical variables (see [33] as a reference text for the subject), with its target configuration space the group manifold of $SU(2)$. The Lagrangian and Hamiltonian formulation are respectively described on the tangent/cotangent bundle of the group.

In the Lagrangian approach the dynamics is defined on the tangent bundle, $TSU(2)$, in terms of an action functional

$$S_0 = \int_{\mathbb{R}} L_0\, dt = -\frac{1}{4}\int_{\mathbb{R}} \mathrm{Tr}\,(\varphi^*(g^{-1}dg) \wedge \underset{H}{*}\varphi^*(g^{-1}dg)) = -\frac{1}{4}\int_{\mathbb{R}} \mathrm{Tr}\,(g^{-1}\dot{g})^2 dt \tag{19.1}$$

[2] Noncommutative gauge theories usually require that the gauge group be enlarged (see for example [26] for a review). The differential calculus itself may be bigger than in the commutative case (see for example [27] for an occurrence of this phenomenon in three dimensions and [28] for an application to two-dimensional gauge theory.

In order to cure nonrenormalizability of noncommutative field theories auxiliary terms have to be added to the action functional, which involve auxiliary parameters. This is the case of simple scalar field theories such as the Grosse-Wulkenhaar model [29], or the translation-invariant model [30].

where $\varphi : t \in \mathbb{R} \to SU(2)$ is the group-valued dynamical variable, while φ^* is the induced pull-back map. $g^{-1}dg = 2i\alpha^k e_k$ is the Maurer-Cartan left-invariant one-form, $e_k = \sigma_k/2$ are the $SU(2)$ generators with σ_k the Pauli matrices, α^k are the basic left-invariant one-forms, $\underset{H}{*}$ denotes the Hodge star operator on the source space $\mathbb{R}$, such that $*_H dt = 1$, and Tr the trace over the Lie algebra. Moreover,

$$g^{-1}\dot{g} \equiv \varphi^*(g^{-1}dg)(\Gamma) \tag{19.2}$$

with $\Gamma = d/dt$ the dynamical field. The model can be regarded as a $(0+1)$-dimensional field theory which is group-valued.

From now on, to simplify the notation, we shall trade $g^{-1}dg$ for its pull-back, and the dynamical variable φ for g, as it is customary in the dynamics of fields over Lie groups. The group manifold being a three-sphere, we can look at it as a submanifold of $\mathbb{R}^4$, satisfying the constraint $(y^0)^2 + \sum_i (y^i)^2 = 1$. It it then straightforward to check that group elements, which have to obey $g^\dagger = g^{-1}$ and $\det g = 1$, can be parameterized according to $g = 2(y^0 e_0 + i y^i e_i)$, with $e_0 = \mathbb{1}/2$. By observing that, in the chosen parametrization

$$g^{-1}\dot{g} = 2i(y^0\dot{y}^i - y^i\dot{y}^0 + \varepsilon^i{}_{jk} y^j \dot{y}^k)e_i \tag{19.3}$$

left generalized velocities $\dot{Q}^i$ may be introduced

$$\dot{Q}^i \equiv (y^0\dot{y}^i - y^i\dot{y}^0 + \varepsilon^i{}_{jk} y^j \dot{y}^k) \tag{19.4}$$

so that $g^{-1}\dot{g} = 2i\dot{Q}^i e_i$. $(Q^i, \dot{Q}^i)$ $i = 1, \ldots, 3$ are therefore tangent bundle coordinates, with Q^i implicitly defined [33]. From right-invariant one-forms one could define right generalized velocities in an analogous way. They give an alternative set of coordinates over the tangent bundle.

The Lagrangian L_0 can be read from the action (19.1). In the chosen coordinates it can be written as:

$$L_0 = \frac{1}{2}\dot{Q}^i \dot{Q}^j \delta_{ij} \tag{19.5}$$

hence describing a free dynamics over the three sphere. In intrinsic formulation, which is especially useful for generalizations, Euler-Lagrange equations of motion can be restated as [33]

$$\mathsf{L}_\Gamma \theta_L - dL_0 = 0 \tag{19.6}$$

with

$$\theta_L = \frac{1}{2}\,\mathrm{Tr}\,[g^{-1}\dot{g}\; g^{-1}dg] = \dot{Q}^i \alpha^j \delta_{ij} \tag{19.7}$$

the Lagrangian one-form and L_Γ the Lie derivative with respect to the dyamical field. With a little calculation we obtain

$$\mathsf{L}_\Gamma \dot{Q}^j \delta_{ji} - \dot{Q}^p \dot{Q}^q \varepsilon_{ip}{}^k \delta_{qk} = \mathsf{L}_\Gamma \dot{Q}^j \delta_{ji} = 0 \tag{19.8}$$

because of the rotation invariance of the product and the complete antisymmetry of the structure constants of $SU(2)$.

Equivalently, we can describe the dynamics on the cotangent bundle, $T^*SU(2)$, in terms of left coordinates (Q^i, I_i) and $I_i = \frac{\partial L_0}{\partial \dot{Q}^i} = \delta_{ij}\dot{Q}^j$ denoting left momenta. As above, an alternative set of fiber coordinates is represented by right momenta, which are obtained from right generalized velocities.

By Legendre transform we obtain:

$$H_0 = [I_i \dot{Q}^i - L_0]_{\dot{Q}^i = \delta^{ij} I_j} = \frac{1}{2}\delta^{ij} I_i I_j \tag{19.9}$$

which is the Hamiltonian of the rigid rotor, in the standard text-books form, with I_i, $i = 1, 2, 3$ the angular momentum components. The dynamics of the IRR is readily obtained by supplementing the Hamiltonian (19.9) with the following Poisson brackets

$$\{y^i, y^j\} = 0 \tag{19.10}$$

$$\{I_i, I_j\} = \varepsilon_{ij}{}^k I_k \tag{19.11}$$

$$\{y^i, I_j\} = \delta^i_j y^0 + \varepsilon^i{}_{jk} y^k \quad \text{or equivalently} \quad \{g, I_j\} = 2ige_j \tag{19.12}$$

which are easily derived from the action with standard techniques [11]. Hence Hamilton equations of motion for the system read

$$\dot{I}_i = 0, \quad g^{-1}\dot{g} = 2iI_i\delta^{ij}e_j$$

namely fiber variables I_i representing the angular momentum are constants of motion, while the orientation of the rotor, which is associated with base space coordinates (y^0, y^i), undergoes a uniform precession. According to (19.11) right rotations are implemented canonically and the Hamiltonian is left invariant.

Analogously, we can deduce that right momenta are canonically realized and conserved as well, hence the model is also left-invariant.

Let us briefly recall some well known facts about the geometric structure of the two carrier spaces considered, namely $TSU(2)$ and $T^*SU(2)$. As manifolds both the bundles are diffeomorphic to the product $S^3 \times \mathbb{R}^3$ and both have the structure of a Lie group, the former being given by the product of the Lie group with the vector space spanned by its Lie algebra, $\mathfrak{su}(2) \simeq \mathbb{R}^3$, the latter by the product of the Lie group with the dual of its Lie algebra, $\mathfrak{su}(2)^* \simeq \mathbb{R}^3$. Although the fibers are diffeomorphic, their geometric structure is dual: tangent bundle coordinates, $\dot{Q}^i$, denote vector fields components, whereas cotangent bundle coordinates, I_i, are components of one-forms. This almost trivial remark will be relevant in next section, where the interesting structure to us will be the semi-direct nature of $T^*SU(2)$ and the Abelian structure of $\mathfrak{su}(2)^*$ will be deformed.

Before closing the section let us mention that already in [13] the phase space of the rigid rotator was generalized to the semi-simple group $SL(2, C)$, by replacing the Abelian subgroup R^3 of the semi-direct product above, with the Borel group $SB(2, \mathbb{C})$, namely, passing to the *double* Lie group of $SU(2)$. In next section we shall review the mathematical construction of Drinfel'd double Lie groups and their relation with the structures of Generalized Geometry. Our generalization will be however different form the one considered in [13].

19.3 Poisson-Lie Groups and the Double Lie Algebra $\mathfrak{sl}(2, \mathbb{C})$

A Poisson-Lie group [10, 34–36] is a Lie group equipped with a Poisson structure which is compatible with the group composition. A typical example is the cotangent bundle of a Lie group, equipped with the natural Kirillov-Souriau-Konstant (KSK) Poisson bracket along the fibers and trivial Poisson bracket on the base manifold. As an example, which is relevant to us, let us consider in detail $T^*SU(2)$. As a group, this is the semi-direct product of $SU(2)$ and the Abelian group $\mathfrak{su}(2)^* \rightleftharpoons \mathbb{R}^3$, with the corresponding Lie algebra given by the semidirect sum $\mathfrak{su}(2) \dot{\oplus} \mathfrak{su}(2)^*$ and Lie bracket:

$$\left[L_i, L_j\right] = i\varepsilon_{ij}{}^k L_k, \qquad \left[T_i, T_j\right] = 0, \qquad \left[L_i, T_j\right] = i\varepsilon_{ij}{}^k T_k. \tag{19.13}$$

It is then a standard procedure to associate with $L_i \in \mathfrak{su}(2)$ linear functions over the dual algebra $\mathfrak{su}(2)^*$, and with $T_i \in \mathfrak{su}(2)^*$ linear functions on $(\mathfrak{su}(2)^*)^* = \mathfrak{su}(2)$. The former correspond to the momenta, I_i, while the latter, being $\mathfrak{su}(2)^*$ Abelian, can be traded directly by coordinate functions over the group manifold, $y^\mu \in C^\infty(G)$. A compatible Poisson structure on the group manifold is thus the one given by (19.10)–(19.12).

Going back to the general case, let us see what are the constraints for the Poisson structure on the group manifold. Its linearization at the unit e of the group provides a Lie algebra structure over the dual algebra $\mathfrak{g}^* = T^*_e(G)$ by the relation

$$[d\xi_1(e), d\xi_2(e)]^* = d\{\xi_1, \xi_2\}(e) \tag{19.14}$$

with $\xi_i \in C^\infty(G)$. The compatibility condition between the Poisson and Lie structures of G yields the relation:

$$\begin{aligned} &\langle [X, Y], [v, w]^* \rangle + \langle \mathrm{ad}^*_v X, \mathrm{ad}^*_Y w \rangle - \langle \mathrm{ad}^*_w X, \mathrm{ad}^*_Y v \rangle \\ &\quad - \langle \mathrm{ad}^*_v Y, \mathrm{ad}^*_X w \rangle + \langle \mathrm{ad}^*_w Y, \mathrm{ad}^*_X v \rangle = 0 \end{aligned} \tag{19.15}$$

with $v, w \in \mathfrak{g}^*, X, Y \in \mathfrak{g}$ and $\mathrm{ad}^*_X, \mathrm{ad}^*_v$ the coadjoint actions of the Lie algebras $\mathfrak{g}, \mathfrak{g}^*$ on each other. This allows one to define a Lie bracket in $\mathfrak{g} \oplus \mathfrak{g}^*$ through the formula:

$$[X+\xi, Y+\zeta] = [X,Y] + [\xi,\zeta]^* - ad^*_X\zeta + ad^*_Y\xi + ad^*_\zeta X - ad^*_\xi Y. \quad (19.16)$$

The symmetry between $\mathfrak{g}$ and $\mathfrak{g}^*$ implies that one has also a Poisson-Lie group G^* with Lie algebra $(\mathfrak{g}^*, [\ ,\ ]^*)$ and a Poisson structure whose linearization at $e \in G^*$ gives the bracket $[\ ,\ ]$. G^* is the dual Poisson-Lie group of G. The Lie group D, associated with the Lie algebra $\mathfrak{d} = \mathfrak{g} \bowtie \mathfrak{g}^*$ is the Drinfel'd double group of both groups, G and G^*, being the construction symmetric.[3] Let us notice that T^*G is an example of a double Lie group, with $G^* = \mathfrak{g}^* = \mathbb{R}^n$ Abelian.

There is a dual algebraic approach to the picture above, mainly due to Drinfel'd [9], which starts from a deformation of the semi-direct sum $\mathfrak{g} \dot{\oplus} \mathbb{R}^n$ into a fully non-Abelian Lie algebra. Let us review the construction for the group $SU(2)$, whose Drinfel'd double is the group $SL(2,\mathbb{C})$ [9].

One starts from the complex Lie algebra $\mathfrak{sl}(2)$, with generators

$$t_1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; \quad t_2 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}; \quad t_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (19.17)$$

satisfying:

$$[t_3, t_1] = 2t_1; \quad [t_3, t_2] = -2t_2; \quad [t_1, t_2] = t_3. \quad (19.18)$$

The real algebra $\mathfrak{sl}(2, C)$ is obtained by considering the complex linear combinations

$$e_1 = \frac{1}{2}(t_1 + t_2) = \frac{\sigma_1}{2}, \quad e_2 = \frac{i}{2}(t_2 - t_1) = \frac{\sigma_2}{2}, \quad e_3 = \frac{1}{2}t_3 = \frac{\sigma_3}{2} \quad (19.19)$$

$$b_i = ie_i \quad i = 1,2,3 \quad (19.20)$$

with Lie brackets

$$[e_i, e_j] = i\varepsilon_{ij}{}^k e_k, \quad [e_i, b_j] = i\varepsilon_{ij}{}^k b_k, \quad [b_i, b_j] = -i\varepsilon_{ij}{}^k e_k \quad (19.21)$$

and $\{e_i\}, i = 1,2,3$, generating the $\mathfrak{su}(2)$ subalgebra.

A different basis can be chosen, by introducing:

$$\tilde{e}^1 = it_1; \qquad \tilde{e}^2 = t_1; \qquad \tilde{e}^3 = \frac{i}{2}t_3, \quad (19.22)$$

which are dual to the generators (19.19), with respect to the scalar product naturally defined on $\mathfrak{sl}(2,\mathbb{C})$ as:

$$\langle u, v\rangle = 2\,\mathrm{Im}[\ \mathrm{Tr}\,(uv)\ ], \quad \forall u, v \in \mathfrak{sl}(2,\mathbb{C}). \quad (19.23)$$

We have indeed

[3] We denote with the symbol $\bowtie$ the Lie algebra structure of $\mathfrak{d}$ as a sum of two non-Abelian, non commuting subalgebras, each one of them acting on its dual.

$$\langle \tilde{e}^i, e_j \rangle = 2\,\mathrm{Im}[\ \mathrm{Tr}\,(\tilde{e}^i e_j)\ ] = \delta^i_j. \tag{19.24}$$

Hence, $\{\tilde{e}^j\}$ span the dual vector space $\mathfrak{su}(2)^*$. This is by itself a Lie algebra, the special Borel subalgebra $\mathfrak{sb}(2,\mathbb{C})$ with Lie brackets:

$$[\tilde{e}^i, \tilde{e}^j] = i f^{ij}{}_k \tilde{e}^k \tag{19.25}$$

and $f^{ij}{}_k = \varepsilon^{ijl}\varepsilon_{l3k}$. Moreover

$$[\tilde{e}^i, e_j] = i\varepsilon^i{}_{jk}\tilde{e}^k + i e_k f^{ki}{}_j. \tag{19.26}$$

Since

$$\langle e_i, e_j \rangle = \langle \tilde{e}^i, \tilde{e}^j \rangle = 0 \tag{19.27}$$

both $\mathfrak{su}(2)$ and $\mathfrak{sb}(2,\mathbb{C})$ are maximal isotropic subspaces of $\mathfrak{sl}(2,\mathbb{C})$ with respect to the scalar product (19.23). We have $\mathfrak{sl}(2,\mathbb{C}) = \mathfrak{su}(2) \bowtie \mathfrak{sb}(2,\mathbb{C})$. Therefore, the Lie algebra $\mathfrak{sl}(2,\mathbb{C})$ can be split into two maximally isotropic dual Lie subalgebras with respect to a bilinear, symmetric, non degenerate form defined on it. The couple $(\mathfrak{su}(2), \mathfrak{sb}(2,\mathbb{C}))$, with the dual structure described above, is a Lie bialgebra and the role of $\mathfrak{su}(2)$ and its dual algebra can be interchanged. The triple $(\mathfrak{sl}(2,\mathbb{C}), \mathfrak{su}(2), \mathfrak{sb}(2,\mathbb{C}))$ is called a *Manin triple* [9].

$D = SL(2,\mathbb{C})$ is thus the *double group* obtained by exponentiating the bialgebra. It may be endowed with a Poisson bracket on the group manifold compatible with the group structure, which we shall consider in Sect. 19.5.2. The two partner groups, $G = SU(2)$ and $G^* = SB(2,\mathbb{C})$ with suitable Poisson brackets, are named *dual groups*.

Besides the scalar product (19.23), there is another non-degenerate, positive-definite scalar product, in $\mathfrak{sl}(2,\mathbb{C})$ given by

$$(u, v) = 2Re[\ \mathrm{Tr}\,(uv)\ ] \qquad \forall u, v \in \mathfrak{sl}(2,\mathbb{C}). \tag{19.28}$$

with new maximal isotropic subspaces which are spanned by:

$$f_i^+ = \frac{1}{\sqrt{2}}(e_i + b_i); \qquad f_i^- = \frac{1}{\sqrt{2}}(e_i - b_i). \tag{19.29}$$

satisfying

$$(f_i^+, f_j^+) = (f_i^-, f_j^-) = 0; \quad (f_i^+, f_j^-) = \delta_{ij}. \tag{19.30}$$

By denoting by C_+ and C_- the two subspaces spanned by $\{e_i\}$ and $\{b_i\}$ respectively, one can notice [6] that the splitting $\mathfrak{d} = C_+ \oplus C_-$ defines a positive definite metric, G, which we shall indicate with double round brackets,

$$((\ ,\ )) := (\ ,\ )_{C_+} - (\ ,\ )_{C_-} \tag{19.31}$$

One has then:

$$((e_i, e_j)) \equiv (e_i, e_j) = \delta_{ij}, ; \qquad ((b_i, b_j)) \equiv -(b_i, b_j) = \delta_{ij}, ;$$
$$((e_i, b_j)) \equiv (e_i, b_j) = 0. \tag{19.32}$$

To summarize, we have introduced two different scalar products on $\mathfrak{sl}(2, \mathbb{C})$, which we shall indicate respectively by η and G. On introducing the double notation

$$e_I = \begin{pmatrix} e_i \\ e^i \end{pmatrix}, \qquad e_i \in \mathfrak{su}(2), \quad e^i \in \mathfrak{sb}(2, \mathbb{C}) \tag{19.33}$$

the scalar product (19.23) may be rewritten as

$$\langle e_I, e_J \rangle = \eta_{IJ} = \begin{pmatrix} 0 & \delta_i^j \\ \delta_j^i & 0 \end{pmatrix}. \tag{19.34}$$

This symmetric inner product has signature (d, d) and therefore defines the non-compact orthogonal group $O(d, d)$, with $d = 3$ in this case.

The Riemannian product (19.32) yields instead:

$$((e_I, e_J)) = G_{IJ} = \begin{pmatrix} \delta_{ij} & \delta_{il}\varepsilon^{jl3} \\ \varepsilon^{il3}\delta_{lj} & \delta^{ij} + \varepsilon^{il3}\delta_{lk}\varepsilon^{jk3} \end{pmatrix}. \tag{19.35}$$

The two metrics can be checked to satisfy the relation:

$$G^T \eta G = \eta \tag{19.36}$$

hence, G is a pseudo-orthogonal $O(3, 3)$ matrix.

19.4 A Model over the Dual Group $SB(2, \mathbb{C})$

Having discussed what may be called an Iwasawa decomposition of the Lorentz universal covering $SL(2, \mathbb{C})$, and having discovered that the dual partner of the special unitary group $SU(2)$ is the special Borel group $SB(2, \mathbb{C})$, it is natural to wonder what could possibly be a natural dynamics on its group manifold and whether the models defined on the partner groups are dual in some precise mathematical sense, inherited from the parent double group.

As carrier space for the dynamics in the Lagrangian (respectively Hamiltonian) formulation we choose therefore the tangent (respectively cotangent) bundle of the group $SB(2, \mathbb{C})$. A suitable action for the system is the following:

$$\tilde{S}_0 = \int_{\mathbb{R}} \tilde{L}_0 \, dt = -\frac{1}{4} \int_{\mathbb{R}} \mathscr{T}r \, [\tilde{\varphi}^*(\tilde{g}^{-1} d\tilde{g} \wedge {}_{H}{*}\tilde{\varphi}^*(\tilde{g}^{-1} d\tilde{g})]$$
$$= -\frac{1}{4} \int_{\mathbb{R}} \mathscr{T}r \, [(\tilde{g}^{-1}\dot{\tilde{g}})(\tilde{g}^{-1}\dot{\tilde{g}})] dt \tag{19.37}$$

with $\tilde{\varphi} : t \in \mathbb{R} \to SB(2, \mathbb{C})$, the group-valued dynamical variable, and $\tilde{\varphi}^*$ the pull-back map. Analogously to the IRR case, $\tilde{g}^{-1} d\tilde{g} = i\beta_k \tilde{e}^k$ represents the Maurer-Cartan left invariant one-form on the group manifold, with β_k the left-invariant basic one-forms, ${}_{H}{*}$ the Hodge star operator on the source space $\mathbb{R}$, such that ${}_{H}{*}dt = 1$. Moreover, as previously, in order to adhere to the notation which is commonly adopted in field theory, we shall identify the dynamical variable $\tilde{\varphi}$ with $\tilde{g}$ for the remainder of this section. As a scalar product in the Lie algebra, which we have indicated with $\mathscr{T}r$, we shall use the one descending form the Riemannian metric G defined on $\mathfrak{sl}(2, \mathbb{C})$ in (19.32), which yields for the $\mathfrak{sb}(2, \mathbb{C})$ generators

$$((\tilde{e}^i, \tilde{e}^j)) = \delta^{ij} + \varepsilon^i{}_{l3} \delta^{lk} \varepsilon^j{}_{k3} \tag{19.38}$$

Let us notice that this is not invariant under right action of the group, because the generators $\tilde{e}^i$ are not Hermitian, while (19.38) can be verified to be equivalent to:

$$((u, v)) \equiv 2\mathrm{Re} \, \mathrm{Tr} \, [(u)^\dagger v]. \tag{19.39}$$

Similarly to the IRR case, the group manifold can be parametrized with $\mathbb{R}^4$ coordinates as $\tilde{g} = 2(u_0 \tilde{e}^0 + i u_i \tilde{e}^i)$, with $u_0^2 - u_3^2 = 1$ and $\tilde{e}^0 = \mathbb{1}/2$. By observing that

$$\tilde{g}^{-1}\dot{\tilde{g}} = 2i(u_0 \dot{u}_i - u_i \dot{u}_0 + f_i{}^{jk} u_j \dot{u}_k)\tilde{e}^i \tag{19.40}$$

the Lagrangian in (19.37) can be rewritten as:

$$\tilde{L}_0 = (u_0 \dot{u}_i - u_i \dot{u}_0 + f_i{}^{jk} u_j \dot{u}_k)(u_0 \dot{u}_r - u_r \dot{u}_0 + f_r{}^{pq} u_p \dot{u}_q)((\tilde{e}^i, \tilde{e}^r)) = \dot{\tilde{Q}}_i \dot{\tilde{Q}}_r h^{ir}$$

with $\dot{\tilde{Q}}_i \equiv u_0 \dot{u}_i - u_i \dot{u}_0 + f_i{}^{jk} u_j \dot{u}_k$ the left generalized velocities and

$$h^{ir} \equiv \delta^{ir} + \varepsilon^{il3} \delta_{ls} \varepsilon^{rs3} \tag{19.41}$$

the metric defined by the scalar product. $(\tilde{Q}_i, \dot{\tilde{Q}}_i)$ are therefore tangent bundle coordinates, with $\tilde{Q}_i$ implicitly defined.

By repeating the analysis already performed for the IRR, one finds the equations of motion:

$$\mathsf{L}_\Gamma(\dot{\tilde{Q}}_j \, i_{\tilde{X}^i} \beta_l) h^{jl} - \mathsf{L}_{\tilde{X}^i} \tilde{L}_0 = \mathsf{L}_\Gamma \dot{\tilde{Q}}_j h^{ji} - \dot{\tilde{Q}}_p \dot{\tilde{Q}}_q f^{ip}{}_k h^{qk} = 0. \tag{19.42}$$

with $\tilde{X}^j$ being the left invariant vector fields generating the right action of $SB(2,\mathbb{C})$. Differently from the IRR case, the second term in the RHS is not vanishing, because the structure constants are not completely antisymmetric. This is to be expected because the Lagrangian is not invariant under right action.

It has to be noticed here that, analogously to the IRR case, one could define the right generalized velocities on the fibers starting from right invariant one-forms, but, differently from that case, the right invariant Lagrangian is not equivalent to the left invariant one.

We can extend the analysis to the cotangent bundle as before, by introducing left coordinates $(\tilde{Q}_i, \tilde{I}^i)$ with $\tilde{I}^i$ the conjugate left momenta $\tilde{I}^j = \frac{\partial \tilde{L}_0}{\partial \dot{\tilde{Q}}_j} = \dot{\tilde{Q}}_r(\delta^{jr} + \varepsilon^j_{l3}\varepsilon^r_{s3}\delta^{ls})$. On inverting for the velocities $\dot{\tilde{Q}}_j = \tilde{I}^i(\delta_{ij} - \frac{1}{2}\varepsilon_i^{p3}\varepsilon_j^{q3}\delta^{pq})$, we obtain the Hamiltonian function:

$$\tilde{H}_0 = [\tilde{I}^j\dot{\tilde{Q}}_j - \tilde{L}]_{\dot{\tilde{Q}}=\dot{\tilde{Q}}(\tilde{I})} = \frac{1}{2}\tilde{I}^i(h^{-1})_{ij}\tilde{I}^j, \tag{19.43}$$

with

$$(h^{-1})_{ij} \equiv (\delta_{ij} - \frac{1}{2}\varepsilon_{ip3}\delta^{pq}\varepsilon_{jq3}). \tag{19.44}$$

On introducing the linear combination: $\tilde{I} = i\tilde{I}^j\tilde{e}^*_j$ with $e_j{}^*(\tilde{e}^i) = \delta^i_j$ we obtain the first order dynamics by means of the following Poisson brackets:

$$\{u_i, u_j\} = 0 \tag{19.45}$$

$$\{\tilde{I}^i, \tilde{I}^j\} = f^{ij}{}_k\tilde{I}^k \tag{19.46}$$

$$\{u_i, \tilde{I}^j\} = \delta^j_i u_0 - f_i{}^{jk}u_k \quad \text{or equivalently} \quad \{\tilde{g}, \tilde{I}^j\} = 2i\tilde{g}\tilde{e}^j \tag{19.47}$$

which are derived from the first order formulation of the action functional (see [11] for details). Specifically we get:

$$\dot{\tilde{I}}^j = \{\tilde{I}^j, \tilde{H}_0\} = f^{jk}_l\tilde{I}^l\tilde{I}^r h^{-1}_{kr} \tag{19.48}$$

which is different from zero, as expected, expressing the non-invariance of the Hamiltonian under right action. Vice-versa, by introducing the right momenta $\tilde{J}^i$ one readily obtains:

$$\dot{\tilde{J}}^j = \{\tilde{J}^j, \tilde{H}_0\} = 0 \tag{19.49}$$

namely, right momenta are constants of the motion and the Hamiltonian is invariant under left action, as it should. Right momenta are therefore conserved, as for the rigid rotator, while left momenta are not.

The same remark as at the end of Sect. 19.2 applies: while the fibers of the tangent bundle $TSB(2,\mathbb{C})$ can be identified, as a vector space, with the Lie algebra $\mathfrak{sb}(2,\mathbb{C}) \simeq \mathbb{R}^3$, with $\dot{\tilde{Q}}_i$ labelling vector fields components, the fibers of the cotangent bundle

$T^*SB(2, C)$ are isomorphic to the dual Lie algebra $\mathfrak{sb}(2, \mathbb{C})^*$.This is isomorphic to $\mathbb{R}^3$ as a vector space, , but $\tilde{I}^j$ are now components of one-forms.

$T^*SB(2, \mathbb{C})$ is identified as a Lie group with the semi-direct product of $SB(2, \mathbb{C})$ and the Abelian group $\mathbb{R}^3$, with Lie algebra the semi-direct sum

$$\left[B_i, B_j\right] = if_{ij}{}^k B_k, \qquad \left[S_i, S_j\right] = 0, \qquad \left[B_i, S_j\right] = if_{ij}{}^k S_k. \tag{19.50}$$

Then, as for the IRR, the non-triviality of the Poisson algebra over the cotangent bundle of the group $SB(2, \mathbb{C})$ reflects the structure of the latter. Again, this is an instance of double Lie group by itself, with trivial Poisson bracket on the group manifold.

Before closing the section, let us summarize the results. We have introduced a model on the dual group of $SU(2)$, the Borel group $SB(2, \mathbb{C})$, whose Hamiltonian dynamics is retrieved in terms of Poisson brackets of KSK type. As we shall see, the Poisson brackets of the momenta $I_i, \tilde{I}^i$ are dually related.

19.5 The Generalized Action

In the previous sections we have introduced two dynamical models on configuration spaces which are dual Lie groups. The Poisson algebras for the respective cotangent bundles, $T^*SU(2)$, $T^*SB(2, \mathbb{C})$, given by

$$\{g, g\} = 0, \quad \{I_i, I_j\} = \varepsilon_{ij}{}^k I_k, \quad \{g, I_j\} = 2ige_j \tag{19.51}$$

$$\{\tilde{g}, \tilde{g}\} = 0, \quad \{\tilde{I}^i, \tilde{I}^j\} = f^{ij}{}_k \tilde{I}^k, \quad \{\tilde{g}, \tilde{I}^j\} = 2i\tilde{g}\tilde{e}^j, \tag{19.52}$$

have both the structure of a semi-direct sum which reflects the semi-direct structure of the Lie algebras $\mathfrak{su}(2)\dot{\oplus}\mathbb{R}^3$ and $\mathfrak{sb}(2, \mathbb{C})\dot{\oplus}\mathbb{R}^3$.

In order to unify the two models within a generalized action, whose configuration space has *double* dimension with respect to the previous ones, let us introduce the configuration space variable $\Phi : t \in \mathbb{R} \to \gamma \in SL(2, \mathbb{C})$. As in previous sections, we shall build an action functional in terms of the geometric structures naturally defined on the tangent space. Therefore, we shall need the pull-back to $\mathbb{R}$ of the left invariant one-form which is defined on the group manifold:

$$\Phi^*(\gamma^{-1}\mathrm{d}\gamma) = \gamma^{-1}\dot{\gamma}\, dt \equiv \dot{\mathbf{Q}}^I e_I \mathrm{d}t \tag{19.53}$$

with $e_I = (e_i, \tilde{e}^i)$ the $\mathfrak{sl}(2, \mathbb{C})$ basis introduced in (19.33) and $\dot{\mathbf{Q}}^I$, the left generalized velocities. Again we adopt the notation which is commonly adopted in field theory and identify the dynamical variable Φ with γ for the remainder of this section. By defining the decomposition $\dot{\mathbf{Q}}^I \equiv (A^i, B_i)$ one has:

$$\gamma^{-1}\dot{\gamma}\, dt = (A^i e_i + B_i \tilde{e}^i)dt$$

where, however, both components are tangent bundle coordinates for $SL(2, C)$. By using the scalar product (19.23), the components of the generalized velocity can be explicitly obtained:

$$A^i = 2\text{Im Tr}\,(\gamma^{-1}\dot{\gamma}\tilde{e}^i); \quad B_i = 2\text{Im Tr}\,(\gamma^{-1}\dot{\gamma}e_i).$$

Having at our disposal two scalar products in the Lie algebra, defined in (19.34), (19.35), the proposed action [11] involves both of them, according to :

$$S = \int_R Ldt = \frac{1}{2}\int_{\mathbb{R}}\left[k_1\langle\gamma^{-1}\mathrm{d}\gamma \stackrel{\wedge}{,} *\gamma^{-1}\mathrm{d}\gamma\rangle + k_2((\gamma^{-1}\mathrm{d}\gamma \stackrel{\wedge}{,} *\gamma^{-1}\mathrm{d}\gamma))\right], \quad (19.54)$$

where k_1, k_2 are real parameters.

Explicitly the generalized Lagrangian reads

$$L = \frac{1}{2}(k\,\eta_{IJ} + G_{IJ})\dot{\mathbf{Q}}^I\dot{\mathbf{Q}}^J \quad (19.55)$$

with

$$k\,\eta_{IJ} + G_{IJ} = \begin{pmatrix} \delta_{ij} & k\delta_i^j + \varepsilon_{3i}{}^j \\ -\varepsilon^i{}_{j3} + k\delta_i^j & \delta^{ij} + \varepsilon^i{}_{l3}\varepsilon^j_{k3}\delta^{lk} \end{pmatrix}$$

the *generalized metric* and the position $k_1/k_2 \equiv k$ has been made. Euler–Lagrange equations read in turn:

$$\mathsf{L}_\Gamma\dot{\mathbf{Q}}^I(k\,\eta_{IJ} + G_{IJ}) - \dot{\mathbf{Q}}^P\dot{\mathbf{Q}}^Q C^K_{IP}(k\,\eta_{QK} + G_{QK}) = 0 \quad (19.56)$$

where C^K_{IP} are the structure constants of $\mathfrak{sl}(2, \mathbb{C})$. The matrix $k\,\eta_{IJ} + G_{IJ}$ is non-singular, provided $k^2 \neq 1$, which will be assumed from now on.

In [11] it has been shown that the Lagrangian of the IRR and of its dual model can be recovered by exploring the global symmetries of the generalized dynamics. If we choose a local parametrization for the elements of the double group $SL(2, \mathbb{C})$: $\gamma = \tilde{g}g$, with $g \in SU(2)$ and $\tilde{g} \in SB(2, \mathbb{C})$, from (19.54) it is easily seen that L is invariant under left and right action of the group $SU(2)$, and under left action of the group $SB(2, \mathbb{C})$. In order to recover the IRR Lagrangian we therefore gauge the $SB(2, \mathbb{C})_L$ global symmetry, by introducing a $SB(2, \mathbb{C})$ gauge connection $\tilde{C} = \tilde{C}_i(t)\tilde{e}^i$:

$$\gamma^{-1}d\gamma \to \gamma^{-1}D_{\tilde{C}}\gamma = (\gamma^{-1}\dot{\gamma} + \gamma^{-1}\tilde{C}\gamma)dt \quad (19.57)$$

and performing the substitution

$$\gamma^{-1}\dot{\gamma} + \gamma^{-1}\tilde{C}\gamma = \gamma^{-1}\dot{\gamma} + \tilde{C}_i\gamma^{-1}\tilde{e}^i\gamma = \mathscr{U}_i\tilde{e}^i + \mathscr{W}^i e_i$$

from which the new variables $\mathscr{U}_i, \mathscr{W}^i$ are easily retrieved. Analogously, in order to obtain the Lagrangian of the dual model we gauge the global $SU(2)_R$ invariance, by

introducing the $SU(2)$ gauge connection $C = C^i(t)e_i$ so to have

$$\gamma^{-1}d\gamma \to \gamma^{-1}D\gamma = \tilde{\mathscr{U}}_i\tilde{e}^i + \tilde{\mathscr{W}}^i e_i. \tag{19.58}$$

By considering each of the gauged Lagrangian functions, $L_{\tilde{C}}$ or L_C and re-expressing them in terms of the new variables, the partition function Z is considered for each of them

$$Z_1 = \int \mathscr{D}g\mathscr{D}\tilde{g}\mathscr{D}\tilde{C}e^{-S_{\tilde{C}}} \tag{19.59}$$

or

$$Z_2 = \int \mathscr{D}g\mathscr{D}\tilde{g}\mathscr{D}Ce^{-S_C} \tag{19.60}$$

and the integration over the gauge potential $\tilde{C}$, respectively C, is performed. Using techniques which are standard in field theory, the integration with respect to the gauge potentials is traded for the integration with respect to $\mathscr{U}_i$, $\tilde{\mathscr{W}}^i$ respectively, so that we are left with half the degrees of freedom of the generalized action (19.54) and we retrieve the IRR model or the dual model, depending on which gauged Lagrangian we started with. We refer for details to [11].

A generalized kinematics in the context of DFT has been considered in [37].

19.5.1 The Hamiltonian Formalism

Let us shortly review the Hamiltonian picture of the doubled dynamics introduced above. Phase space is now $T^*SL(2,\mathbb{C})$ and left generalized momenta associated with fiber coordinates are represented by:

$$\mathbf{P}_I = \frac{\partial L}{\partial \dot{\mathbf{Q}}^I} = (\eta_{IJ} + k\, G_{IJ})\dot{\mathbf{Q}}^J \tag{19.61}$$

The Hamiltonian reads then:

$$H = (\mathbf{P}_I\dot{\mathbf{Q}}^I - L)_{\mathbf{P}} = \frac{1}{2}[(\eta + k\, G)^{-1}]^{IJ}\mathbf{P}_I\mathbf{P}_J \tag{19.62}$$

with

$$[(\eta + k\, G)^{-1}]^{IJ} = \frac{1}{2}(1-k^2)^{-1}\begin{pmatrix} \delta^{ij} + \varepsilon^i_{l3}\varepsilon^j_{k3}\delta^{lk} & -\varepsilon^i{}_{j3} - k\delta^i_j \\ \varepsilon_i{}^{j3} - k\delta^j_i & \delta_{ij} \end{pmatrix}. \tag{19.63}$$

From (19.61) one can explicitly write the generalized momenta $\mathbf{P}_I$ in terms of the components of $\dot{\mathbf{Q}}^I \equiv (A^i, B_j)$, thus finding:

$$\mathbf{P}_I \equiv (I_i, \tilde{I}^i) = \left(\delta_{ij}A^j + (k\delta^j_i + \varepsilon^{j3}_i)B_j, (k\delta^i_j - \varepsilon^i_{j3})A^j + [\delta^{ij} + \delta^{lk}\varepsilon^i_{l3}\varepsilon^j_{k3}]B_j\right). \tag{19.64}$$

In terms of the components $I_i, \tilde{I}^j$, it turns out that:

$$H = \frac{1}{2}(1-k^2)^{-1}\left[(1-k^2)\delta^{ij}I_iI_j + \delta_{ij}(\tilde{I}^i - I_s(k\delta^{si} + \varepsilon^{si}{}_3))(\tilde{I}^j - I_r(k\delta^{rj} + \varepsilon^{rj}{}_3))\right] \tag{19.65}$$

In order to obtain the Hamilton equations for the generalized model on the Drinfel'd double, one can proceed as in the previous sections with the determination of Poisson brackets from the first-order action functional [11], which yields:

$$\{I_i, I_j\} = \varepsilon_{ij}{}^k I_k \tag{19.66}$$

$$\{\tilde{I}^i, \tilde{I}^j\} = f^{ij}{}_k \tilde{I}^k \tag{19.67}$$

$$\{I_i, \tilde{I}^j\} = \varepsilon^j{}_{il}\tilde{I}^l - I_l f^{lj}{}_i \quad \{\tilde{I}^i, I_j\} = -\varepsilon^i{}_{jl}\tilde{I}^l + I_l f^{li}{}_j \tag{19.68}$$

while the Poisson brackets between momenta and configuration space variables $g, \tilde{g}$ are unchanged with respect to $T^*SU(2), T^*SB(2,\mathbb{C})$. We refer to [11] for details.

Poisson brackets may be written in compact form:

$$\{\mathbf{P}_I, \mathbf{P}_J\} = C^K_{IJ}\mathbf{P}_K \tag{19.69}$$

with C^K_{IJ} the structure constants specified above. Thus we have, for Hamilton equations of motion:

$$\frac{d}{dt}\mathbf{P}_I = \{\mathbf{P}_I, \widehat{H}\} = [(\eta + k\,G)^{-1}]^{JK}\{\mathbf{P}_I, \mathbf{P}_J\}\mathbf{P}_K = [(\eta + k\,G)^{-1}]^{JK}C^L_{IJ}\mathbf{P}_L\mathbf{P}_K \tag{19.70}$$

which is not zero, consistently with (19.56) and expresses the non-invariance of the Hamiltonian under right $SL(2,\mathbb{C})$ action.

19.5.2 Poisson Brackets

The Poisson brackets (19.66)–(19.68) among fiber coordinate functions of $T^*SL(2,\mathbb{C})$ have the structure of a Lie bi-algebra, with the mixed bracket realizing the adjoint action of each algebra on the other one. Therefore, they can be regarded as a deformation of those defined on the cotangent bundle of either partner group, as stated in (19.10)–(19.12), or in (19.45)–(19.47).

It is possible to show that (19.66)–(19.68) may be derived from a Poisson bracket on the group manifold of $SL(2,\mathbb{C})$, by linearization at the identity of the group, as in (19.14).

Before commenting on that, let us first consider Poisson brackets introduced long time ago in [10, 34] in the form

$$\{\gamma_1, \gamma_2\} = -\gamma_1\gamma_2 r^* - r\gamma_1\gamma_2 \tag{19.71}$$

Here $\gamma_1 = \gamma \otimes 1$, $\gamma_2 = 1 \otimes \gamma_2$ while $r \in \mathfrak{d} \otimes \mathfrak{d}$ is the classical Yang-Baxter matrix:

$$r = \tilde{e}^i \otimes e_i \tag{19.72}$$

satisfying the modified Yang–Baxter equation

$$[r_{12}, r_{13} + r_{23}] + [r_{13}, r_{23}] = h$$

with $r_{12} = \tilde{e}^i \otimes e_i \otimes \mathbb{1}$, $r_{13} = \tilde{e}^i \otimes \mathbb{1} \otimes e_i$, $r_{23} = \mathbb{1} \otimes \tilde{e}^i \otimes e_i$ and $h \in \mathfrak{d} \otimes \mathfrak{d} \otimes \mathfrak{d}$ an adjoint invariant element in the enveloping algebra. The matrix

$$r^* = -e_i \otimes \tilde{e}^i \tag{19.73}$$

is also solution of the Yang-Baxter equation. On writing γ as $\gamma = \tilde{g}g$ it can be easily checked that (19.71) is compatible with the following choice

$$\{g_1, g_2\} = [r^*, g_1 g_2], \tag{19.74}$$
$$\{\tilde{g}_1, g_2\} = -\tilde{g}_1 r g_2 \tag{19.75}$$
$$\{\tilde{g}_1, \tilde{g}_2\} = -[r, \tilde{g}_1\tilde{g}_2], \tag{19.76}$$

with $g_1 = g \otimes \mathbb{1}$, $g_2 = \mathbb{1} \otimes g$, $\tilde{g}_1 = \tilde{g} \otimes \mathbb{1}$ and $\tilde{g}_2 = \mathbb{1} \otimes \tilde{g}$. Equations (19.74), (19.76) are the so-called Sklyanin brackets [38] on $C^\infty(G)$, $C^\infty(G^*)$ respectively, which make both groups into Poisson–Lie groups, according to the definition we have given in Sect. 19.3.

Let us sketch how to recover (19.10)–(19.12) when passing from the double group $SL(2, \mathbb{C})$ to either of the cotangent bundles. In order to recover the Poisson algebra for $T^*SU(2)$, one has to rescale the matrix r and the group elements of $SB(2, \mathbb{C})$ by a real parameter λ. By expanding up to first order, $\tilde{g}(\lambda) = e^{i\lambda I_i \tilde{e}^i} = 1 + i\lambda I_i \tilde{e}^i + \mathscr{O}(\lambda^2)$ and replacing into (19.76) we obtain:

$$\{\tilde{g}_1, \tilde{g}_2\} = \simeq -\lambda^2 \tilde{e}^i \otimes \tilde{e}^j \{I_i, I_j\} + \mathscr{O}(\lambda^3),$$

which has to be equated to

$$[r, \tilde{g}_1\tilde{g}_2] \simeq -\lambda^2 I_k \varepsilon^k_{ij} e_i \otimes e_j + \mathscr{O}(\lambda^3) \tag{19.77}$$

thus yielding

$$\{I_i, I_j\} = \varepsilon^k_{ij} I_k. \tag{19.78}$$

As for (19.75) in order to compute its l.h.s. we use the parametrization $g = y^0\sigma_0 + iy^i\sigma_i$, so that, up to first order in λ

$$\{\tilde{g}_1, g_2\} = 2i\lambda \left(\{I_i, y^0\}\tilde{e}^i \otimes e_0 + i\{I_i, y^j\}\tilde{e}^i \otimes e_j\right) + O(\lambda^2) \tag{19.79}$$

while for the r.h.s.

$$-\tilde{g}_1 r g_2 \simeq -\lambda(y^0\tilde{e}^k \otimes e_k + iy^j\tilde{e}^k \otimes (\delta_{kj}e_0 + i\varepsilon^i_{kj}e_i) \tag{19.80}$$

thus yielding

$$\{I_i, y^0\} = -y^j\delta_{ij}$$
$$\{I_i, y^j\} = y^0\delta^j_i - y^k\varepsilon^j_{ki}$$

where the first one is compatible with the second one, by using $(y^0)^2 = 1 - \sum_k y^k y^k$. Finally, on considering (19.74), and rescaling r^* by some parameter, we observe that the LHS doesn't depend on λ whereas the RHS does. Therefore we get

$$\{y^0, y^j\} = \{y^i, y^j\} = 0 + O(\lambda). \tag{19.81}$$

Thus, (19.78), (19.81), (19.81) reproduce correctly the canonical Poisson brackets on the cotangent bundle $T^*SU(2)$.

The Poisson brackets for the cotangent bundle $T^*SB(2, \mathbb{C})$ are obtained in complete analogy, when considering r^* as an independent solution of the Yang-Baxter equation

$$\rho = -\mu e_k \otimes \tilde{e}^k \tag{19.82}$$

and expanding $g \in SU(2)$ as a function of the parameter μ

$$g = \mathbb{1} + i\mu\tilde{I}^i e_i + O(\mu^2). \tag{19.83}$$

Let us go back to the fully non-Abelian Poisson algebra represented by (19.66)–(19.68). This is in turn obtained by linearizing the following Poisson bracket [10]:

$$\{\gamma_1, \gamma_2\} = \frac{\lambda}{2}\left[\gamma_1(r^* - r)\gamma_2 - \gamma_2(r^* - r)\gamma_1\right]. \tag{19.84}$$

Indeed, on expanding $\gamma \in D$ as $\gamma = \mathbb{1} + i\lambda I_i\tilde{e}^i + i\lambda\tilde{I}^i e_i$ and rescaling r, r^* by the same parameter λ, we get, on the l.h.s. of (19.84),

$$\{\gamma_1, \gamma_2\} = -\lambda^2\left(\{I_i, I_j\}\tilde{e}^i \otimes \tilde{e}^j + \{\tilde{I}^i, \tilde{I}^j\}e_i \otimes e_j + \{I_i, \tilde{I}^j\}(\tilde{e}^i \otimes e_j - e_j \otimes \tilde{e}^i)\right)$$

while, on the r.h.s. of the same equation:

$$-\lambda^2\left(I_s\varepsilon^s_{ij}\tilde{e}^i \otimes \tilde{e}^j + \tilde{I}^s f_s{}^{ij}e_i \otimes e_j + I_s f_i{}^{sj}(\tilde{e}^i \otimes e_j - e_j \otimes \tilde{e}^i) + \tilde{I}^s\varepsilon^j_{si}(\tilde{e}^r \otimes e_j - e_j \otimes \tilde{e}^i)\right).$$

By equating the two results we arrive at:

$$\{I_i, I_j\} = \varepsilon_{ij}{}^k I_k$$
$$\{\tilde{I}^i, \tilde{I}^j\} = f^{ij}{}_k \tilde{I}^k$$
$$\{I_i, \tilde{I}^j\} = -f_i^{jk} I_k - \tilde{I}^k \varepsilon_{ki}{}^j$$

which is what we wanted to prove.

To summarize, all brackets we have employed throughout the paper are related either to the double structure of $SL(2, \mathbb{C})$ or to the Poisson-Lie nature of the dual partners of the Iwasawa decomposition, $SU(2)$, $SB(2, \mathbb{C})$. The final, interesting question which one could address concerns the nature of symmetries of the physical systems considered, which is the subject of next subsection.

19.5.2.1 Poisson-Lie Simmetries

We closely follow [13] for the forthcoming discussion. In particular we want to discuss to what extent the models possess Poisson-Lie symmetries. Poisson-Lie symmetries are Lie group transformations implemented on the carrier space of the dynamics via group multiplication, which, in general, are not canonical transformations as they need not preserve the symplectic structure. However, if the Poisson structure is of the form (19.71) with carrier space D itself, or (19.74), (19.76) if we are looking at G, G^* respectively, Poisson brackets can be made invariant if the parameters of the group of transformations are imposed to have nonzero Poisson brackets with themselves. Group multiplication is then said to correspond to a Poisson map. We have for example, for the right transformations of G on D,

$$\gamma \to \gamma h, \ h \in G, \ \gamma \in D \tag{19.85}$$

and the left action of G^* on D,

$$\gamma \to \tilde{h}\gamma, \ h^* \in G^* \ \ \gamma \in D. \tag{19.86}$$

In terms of the coordinates $(\tilde{g}, g)$ this implies

$$g \to gh, \quad \tilde{g} \to \tilde{g}, \tag{19.87}$$

for the former and

$$g \to g, \quad \tilde{g} \to \tilde{h}\tilde{g}, \tag{19.88}$$

for the latter. By themselves these transformations do not preserve the Poisson brackets (19.74)–(19.76). But they can be made to be invariant if we require that the parameters of the transformation, h, have the following Poisson brackets

$$\{h_1, h_2\} = [r^*, \ h_1 h_2], \tag{19.89}$$

and zero Poisson brackets with g and $\tilde{g}$. Then $SU(2)$ right multiplication is a Poisson map and (19.85) corresponds to a Poisson Lie group transformation. For (19.86) to be a Poisson Lie group transformation, $\tilde{h}$ must have the following Poisson bracket with itself

$$\{\tilde{h}_1, \tilde{h}_2\} = -[r,\ \tilde{h}_1\tilde{h}_2], \tag{19.90}$$

and zero Poisson brackets with g and $\tilde{g}$. Since the right-hand-sides of (19.89) and (19.90) vanish in the limit $\lambda \to 0$, the transformations (19.85) and (19.86) become canonical in the limit.
Moreover, Poisson brackets (19.74)–(19.76) are invariant under the simultaneous action of both G and G^* via (19.85) and (19.86), if we assume that

$$\{\tilde{h}_1, h_2\} = 0. \tag{19.91}$$

By comparing with (19.75) we conclude that the algebra of the observables g and $\tilde{g}$ is different from the algebra of the symmetries parametrized by h and $\tilde{h}$. Therefore, dynamics on the group manifold of $SL(2, \mathbb{C})$ and on the two partner groups $SU(2)$ and $SB(2, \mathbb{C})$ possesses Poisson-Lie group symmetries, when endowed with the above mentioned brackets.

Let us go back to the symplectic structures of the IRR and the dual model, respectively given by (19.11) and (19.46). We have seen in Sect. 19.5.2 that the former is obtained from (19.76) while the latter is obtained from (19.74), for small (but non-zero) value of the parameters λ and μ. Therefore momentum variables of each model inherit their Poisson brackets from the Poisson-Lie structure of the dual group, which in turn exhibits Poisson-Lie symmetry according to the definition we have recalled above. It is only in this way that Poisson–Lie symmetry manifests itself in the models considered.[4]

19.6 Conclusions

We have used the well established notion of Poisson–Lie groups and Drinfel'd double to understand in a clear geometric setting concepts such as target-space duality, generalized geometry and doubling of degrees of freedom. To this, we have chosen as a toy model a simple dynamics on the group manifold of $SU(2)$, which is that of the isotropic rigid rotor, inspired by an existing description of the model on the double Lie group $SL(2, C)$ [13]. We have introduced a new dynamical model which is dual to the standard IRR and we have used the Drinfel'd double of the group $SU(2)$ as the configuration space for the dynamics of a generalized model, with doubled degrees of freedom. Moreover, we have shown that, from the generalized action, the

[4]The issue of Poisson–Lie symmetries for dynamics such as those discussed in this paper is further elucidated and better understood in the context of field theory in a recent paper [12], where a higher dimensional analogue of the IRR is analyzed. We refer to that for details.

usual description with half the degrees of freedom, can be recovered by gauging one of its symmetries. This model represents an ideal arena to analyze in a simple context the meaning to physics of generalized and doubled geometry structures.

The simple model of the IRR is especially interesting as a toy model for field theories with non-trivial target spaces such as Principal Chiral Models. The latter are non-linear sigma models defined on some $d+1$ dimensional space–time in terms of group–valued fields, $\varphi : R^{d+1} \to SU(N)$, hence representing a d dimensional generalization of the IRR model. For $d = 1$ and the target space reduced to some coset space of the group, these models are also of interest for string theory.

By simply looking at the action functional

$$S = \frac{1}{2} \int_{\mathbb{R}^n} \mathrm{Tr}\,[\varphi^*(g^{-1}\mathrm{d}g) \wedge \underset{H}{*}\varphi^*(g^{-1}\mathrm{d}g)], \tag{19.92}$$

with now $\varphi : \mathbb{R}^{d+1} \to g \in SU(N)$ and $\underset{H}{*}$ the Hodge star operator on $\mathbb{R}^{d+1}$, their analogy with the IRR appears evident. Indeed, in [12] the analysis performed here has been generalized, starting from an alternative description of Principal Chiral Models given in [39–42] (also see [43, 44] where sigma models are studied in the DFT context) and the symmetries have been discussed.

Acknowledgements P. V. acknowledges support by COST (European Cooperation in Science and Technology) in the framework of COST Action MP1405 QSPACE.

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Chapter 20
Loops of Legendrians in Contact 3-Manifolds

Eduardo Fernández, Javier Martínez-Aguinaga and Francisco Presas

Abstract We study homotopically non-trivial spheres of Legendrians in the standard contact $\mathbb{R}^3$ and $\mathbb{S}^3$. We prove that there is a homotopy injection of the contactomorphism group of $\mathbb{S}^3$ into some connected components of the space of Legendrians induced by the natural action. We also provide examples of loops of Legendrians that are non-trivial in the space of formal Legendrians, and thus non-trivial as loops of Legendrians, but which are trivial as loops of smooth embeddings for all the smooth knot types.

20.1 Introduction

This small note summarizes the current understanding of the topology of the spaces of Legendrian embeddings in the 3-dimensional case just using classical invariants. The study of the connected components of those spaces has been a classical topic in the Contact Topology literature [3, 4, 6–8, 14, 16].

Here we focus on the higher dimensional homotopy groups, in particular in the fundamental group. We define invariants and provide partial classifications by considering the space of Legendrian embeddings as a subspace of the space of formal Legendrian embeddings. Then, we provide non-trivial homotopy elements considered as homotopy classes in the space of formal Legendrian embeddings and clearly

E. Fernández · J. Martínez-Aguinaga
Universidad Complutense de Madrid, Facultad de Matemáticas,
C. Nicolás Cabrera, 13-15, 28049 Madrid, Spain
e-mail: edufdezfuertes@gmail.com

J. Martínez-Aguinaga
e-mail: xabi.martinez.aguinaga@gmail.com

E. Fernández (✉) · J. Martínez-Aguinaga · F. Presas
Instituto de Ciencias Matemáticas CSIC-UAM-UC3M-UCM,
C. Nicolás Cabrera, 13-15, 28049 Madrid, Spain
e-mail: fpresas@icmat.es

G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5_20

we conclude that the classes are non-trivial in the space of Legendrian embeddings. Do note that, in dimension 3, there are not known examples of non-trivial spheres of Legendrian embeddings that are trivial as spheres of formal Legendrian embeddings, see [9].

20.2 Preliminaries on Contact 3-Manifolds

We introduce the basic terminology in 3-dimensional contact topology that we are going to use. For further details see [10].

20.2.1 Contact 3-Manifolds

Definition 1 Let M be a 3-manifold. A plane field $\xi \subseteq TM$ is said to be a *contact distribution* if it is everywhere non integrable, i.e. locally ξ can be regarded as the kernel of a 1-form $\alpha \in \Omega^1(M)$ such that

$$\alpha \wedge d\alpha \neq 0. \tag{20.1}$$

The pair (M, ξ) is a *contact* 3*-manifold*.

Assume that ξ is *coorientable*. Thus, $\xi = \ker \alpha$ for some 1-form $\alpha \in \Omega^1(M)$ satisfying (20.1). The election of α is unique up to a conformal factor. From now on, we will focus in the case of *cooriented contact structures*.

A diffeomorphism $f : (M_1, \xi_1) \to (M_2, \xi_2)$ between two contact 3-manifolds, such that $f_*\xi_1 = \xi_2$ is said to be a *contactomorphism*. Denote by $\mathrm{Cont}(M, \xi)$ the group of contactmorphisms from (M, ξ) to itself. Locally any two contact 3-manifolds are contactomorphic, this is the content of *Darboux's Theorem* (see [10], Theorem 2.5.1).

The *Reeb vector field* associated to a contact form α defining a contact manifold $(M, \xi = \ker \alpha)$ is the unique vector field R_α defined by the conditions $\alpha(R_\alpha) \equiv 1$ and $i_{R_\alpha} d\alpha \equiv 0$.

Example 1 The two basic examples that we are going to study in this note are the following

(i) The standard contact structure on $\mathbb{R}^3(x, y, z)$ given by $\xi_{\mathrm{std}} = \ker(dz - ydx)$.
(ii) The standard contact structure on $\mathbb{S}^3 \subseteq \mathbb{C}^2(z_1, z_2)$ given by $\xi_{\mathrm{std}} = T\mathbb{S}^3 \cap iT\mathbb{S}^3 = \ker(\frac{i}{2}\sum_j z_j d\bar{z}_j - \bar{z}_j dz_j)$, where $i : T\mathbb{C}^2 \to T\mathbb{C}^2$ denotes the standard complex structure on $\mathbb{C}^2$. It follows that $(\mathbb{R}^3, \xi_{\mathrm{std}})$ is contactomorphic to $(\mathbb{S}^3 \backslash \{p\}, \xi_{\mathrm{std}|_{\mathbb{S}^3 \backslash \{p\}}})$, for any point $p \in \mathbb{S}^3$ (see [10], Proposition 2.1.8). This justifies the notation.

20.3 Legendrian Submanifolds

Following [7, 10] we introduce the notion of *Legendrian submanifold* of a contact manifold. We define the (formal) *classical invariants*. We also introduce two (formal) invariants for loops of Legendrians.

20.3.1 Legendrian Submanifolds

Definition 2 Let (M, ξ) be a contact 3-manifold. An embedded oriented circle $L \subseteq M$ is said to be *Legendrian* if $TL \subseteq \xi$. A *Legendrian embedding* is any embedding that parametrizes a Legendrian submanifold.

Denote by $\widehat{\mathfrak{Leg}}(M, \xi)$ the space of Legendrian submanifolds of (M, ξ) and by $\mathfrak{Leg}(M, \xi)$ the space of Legendrian embeddings of (M, ξ). Note that $\widehat{\mathfrak{Leg}}(M, \xi) = \mathfrak{Leg}(M, \xi)/\operatorname{Diff}^+(\mathbb{S}^1)$.

A key result in the theory of Legendrian submanifolds is the *Weinstein's Tubular Neighbourhood Theorem* (see [10], Corollary 2.5.9) which asserts that two diffeomorphic Legendrians have contactomorphic neighbourhoods. Thus, any Legendrian circle L in a contact 3-manifold has a tubular neighbourhood contactomorphic to a tubular neighbourhood of $\mathbb{S}^1 \times \{0\} \subseteq (\mathbb{S}^1 \times \mathbb{R}^2(\theta, (x, y)), \ker(\cos\theta dx - \sin\theta dy))$.

20.3.1.1 Projections

There are two distinguished projections $\pi : \mathbb{R}^3 \to \mathbb{R}^2$ that are useful in the study of Legendrians. When projecting onto $\mathbb{R}^2$ via the two projections that we will define, each embedding is mapped to a unique curve in $\mathbb{R}^2$. Nevertheless, the converse results are partially true. We can recover a unique Legendrian curve in $(\mathbb{R}^3, \xi_{\text{std}})$ from curves in $\mathbb{R}^2$ satisfying certain conditions.

Definition 3 We define the *Lagrangian projection* as

$$\begin{aligned} \pi_L : \quad \mathbb{R}^3 &\longrightarrow \mathbb{R}^2 \\ (x, y, z) &\longmapsto (x, y). \end{aligned}$$

This projection has the property that maps immersed Legendrian curves in $(\mathbb{R}^3, \xi_{\text{std}})$ to immersed curves in $\mathbb{R}^2$. In addition, the z-coordinate can be recovered by integration:

$$z(t_1) = z(t_0) + \int_{t_0}^{t_1} y(s)x'(s)ds.$$

Thus, in order for a closed curve in $\mathbb{R}^2$ to lift to a closed Legendrian, it is necessary that the closed immersed disk that bounds the curve has zero (signed) area.

On the other hand we have:

Definition 4 We define the *front projection* as

$$\begin{aligned} \pi_F : \quad \mathbb{R}^3 &\longrightarrow \mathbb{R}^2 \\ (x, y, z) &\longmapsto (x, z). \end{aligned}$$

We can recover the y-coordinate by differentiating:

$$y(s) = \frac{z'(s)}{x'(s)}.$$

The cases $x'(s_0) = z'(s_0) = 0$ are allowed as soon as the limit is well defined.

20.3.2 Classical Invariants

There are three *classical invariants* of Legendrian embeddings that we will introduce (for simplicity) only in the context of $(\mathbb{R}^3, \xi_{\text{std}})$ and $(\mathbb{S}^3, \xi_{\text{std}})$. The first one is the *smooth knot type of the embedding*, which is purely topological.

Let (M, ξ) be $(\mathbb{R}^3, \xi_{\text{std}})$ or $(\mathbb{S}^3, \xi_{\text{std}})$. Let $\gamma \in \mathfrak{Leg}(M, \xi)$ be a Legendrian embedding. We call *contact framing* to the trivialization of its normal bundle $\nu(\gamma)$ given by the Reeb vector field along the knot. We call *topological framing* of γ to the framing $\mathcal{F}_{\pi}$ of $\nu(\gamma)$ defined by any Seifert surface of γ.

Definition 5 The *Thurston-Bennequin* invariant of γ, denoted by $\text{tb}(\gamma)$, is the twisting of the contact framing with respect to the topological framing.

Fix a global trivialization of ξ, this election is unique up to homotopy since $\pi_0(\mathcal{M}\mathfrak{aps}(M, \mathbb{S}^1)) = 0$ for the two particular manifolds that we are studying. Thus, the derivative of the Legendrian embedding defines a map $\gamma' : \mathbb{S}^1 \to \mathbb{R}^2 \backslash \{0\}$.

Definition 6 The *rotation number* of $\gamma \in \mathfrak{Leg}(M, \xi)$ is

$$\text{Rot}(\gamma) = \deg \gamma'.$$

It follows that the rotation number is well defined and independent of the trivialization of ξ. In the case that ξ is non-trivial, we can define the rotation number for null-homologous knots by just taking a Seifert surface Σ on a fixed homology class and selecting a framing for $\xi_{|\Sigma}$ that induces a framing over the boundary by restriction. The induced framing on $\xi_{|\gamma}$ is independent of the choice (see [10], Proposition 3.5.15).

There is an important result relating the three classical invariants of Legendrian embeddings in $(\mathbb{R}^3, \xi_{\text{std}})$ and $(\mathbb{S}^3, \xi_{\text{std}})$.

Proposition 1 (Bennequin's inequality, [1]) *Let $\chi(\Sigma)$ denote the Euler characteristic of a Seifert surface Σ for the Legendrian embedding γ. Then the following inequality holds:*

$$\mathrm{tb}(\gamma) + |\mathrm{Rot}(\gamma)| \leq -\chi(\Sigma). \tag{20.2}$$

20.3.3 Invariants for Loops of Legendrian Embeddings

We consider parametrized loops, when we quotient by the parameter we explicitely mention it. Let (M, ξ) be $(\mathbb{R}^3, \xi_{\mathrm{std}})$ or $(\mathbb{S}^3, \xi_{\mathrm{std}})$. We can also define certain (formal) invariants for loops of Legendrian embeddings γ^θ in $\mathfrak{Leg}(M, \xi)$. The first invariant is the *homotopy class of the loop* of smooth embeddings, i.e. $[\gamma^\theta] \in \pi_1\left(\mathfrak{Emb}(\mathbb{S}^1, M)\right)$, where $\mathfrak{Emb}(N_1, N_2)$ denotes the space of embeddings of a manifold N_1 into another manifold N_2.

The second invariant for loops of Legendrians embeddings is the following.

Definition 7 The *rotation number of the loop γ^θ* is

$$\mathrm{Rot}_{\pi_1}(\gamma^\theta) = \deg(\theta \mapsto (\gamma^\theta)'(0)).$$

In order to define a different invariant, we assume that there exists a loop of Seifert surfaces Σ^θ for γ^θ. Thus, we have a *loop* of topological framings for $\nu(\gamma^\theta)$. By means of the Reeb vector field, we can understand this loop as a $\mathcal{F}^\theta_\pi : \mathbb{S}^1 \to \mathbb{R}^2 \backslash \{0\}$.

Definition 8 The *Thurston-Bennequin number of the loop γ^θ* is

$$\mathrm{tb}_{\pi_1}(\gamma^\theta) = -\deg(\theta \to \mathcal{F}^\theta_\pi(0)).$$

The Thurston-Bennequin number is not necessarily well defined for all the loops of Legendrian embeddings, since we are assuming that we have a loop of topological framings. The key point is the existence and uniqueness of such a loop.

Assume that a loop of smooth embeddings γ^θ is homotopically trivial, i.e. there is γ^z, $z \in \mathrm{d}$, whose boundary is γ^θ. Thus, there is a unique topological framing on $\gamma^z_{|z=0}$ induced by any choice of Seifert surface. This induces a unique 1-parametric family of topological framings on the loop γ^θ. Now, assume that we have a 2-sphere S of smooth embeddings. If we understand it as the union of two disks we get by the previous construction two possibly different topological framings for the equator γ^θ. The difference between the two loops is measured by an integer $d(S)$. We conclude that we have a well defined morphism of abelian groups $d : \pi_2(\mathfrak{Emb}(\mathbb{S}^1, M)) \to \mathbb{Z}$; $S \mapsto d(S)$. Obviously $\mathrm{Image}(d) = k_0\mathbb{Z}$ for some integer k_0.

Recall that there is a natural left action of $\mathrm{Diff}^+(M)$ on $\mathfrak{Emb}(\mathbb{S}^1, M)$. Denote by $\Phi_\gamma : \mathrm{Diff}^+(M) \to \mathfrak{Emb}(\mathbb{S}^1, M)$ the orbit of an embedding γ under the action.

We can state the following proposition that is obviously true by the previous discussion.

Proposition 2 *Let γ^θ be a loop Legendrian embeddings. In any of the two following cases* tb_{π_1} *is a well defined invariant:*

(A) If $\pi_1(\Phi_\gamma)$ is an monomorphism and $[\gamma^\theta] \in \mathrm{Image}(\pi_1(\Phi_\gamma))$ or
(B) γ^θ is trivial as a loop of smooth embeddings. In this case $\mathrm{tb}_{\pi_1}(\gamma^\theta) \in \mathbb{Z}/k_0\mathbb{Z}$.

Remark 1 Assume that γ^θ satisfies condition (A) and condition (B). Then, $k_0 = 0$ and $\mathrm{tb}^B_{\pi_1}(\gamma^\theta) = \mathrm{tb}^A_{\pi_1}(\gamma^\theta) \in \mathbb{Z}$. The reason is that condition (B) provides a capping disk $\gamma^{r,\theta}$ for γ^θ. Now the segment γ^{r,θ_0}, by the *Isotopy Extension Theorem,* can be represented by a segment of diffeomorphisms Ψ_{r,θ_0}, i.e. $\Psi_{0,\theta_0} = \mathrm{Id}$ and $\Psi_{r,\theta_0}(\gamma^0) = \gamma^{r,\theta_0}$. Thus, $\Psi_{1,\theta}(\gamma^0) = \gamma^\theta$ and the two definitions do coincide. This also implies $k_0 = 0$. For this reason, we do not specify if we are considering the type (A) invariant or the type (B) invariant in the discussion that follows.

Finally, we can state the following useful formulas.

Proposition 3 *Let γ^θ be a loop of Legendrian embeddings. For each $k \in \mathbb{Z}$ define the reparametrizations $\gamma^{\theta,k}(t) := \gamma^\theta(t - k\theta)$. Then,*

(i) $\mathrm{Rot}_{\pi_1}(\gamma^{\theta,k}) = \mathrm{Rot}_{\pi_1}(\gamma^\theta) - k\,\mathrm{Rot}(\gamma^0)$,
(ii) $\mathrm{tb}_{\pi_1}(\gamma^{\theta,k}) = \mathrm{tb}_{\pi_1}(\gamma^\theta) - k\,\mathrm{tb}(\gamma^0)$, *whenever the* tb_{π_1} *is well defined for both loops.*

Remark 2 Hatcher's work about knot spaces in $\mathbb{S}^3$ implies that tb_{π_1} is well defined for many cases:

- The connected component $\mathfrak{Emb}_0(\mathbb{S}^1, \mathbb{S}^3)$ of the trivial embedding has the homotopy type of $V_{4,2}$, the space of parametrized great circles (see [11], Appendix: Equivalence (20.6)). Note that, $\pi_1(V_{4,2}) = 0$ and $\pi_2(V_{4,2}) \cong \mathbb{Z}$. In this case $\mathrm{tb}_{\pi_1} \in \mathbb{Z}$ is always defined since $k_0 = 0$. Indeed, consider $\mathbb{S}^3$ as a submanifold of the quarternions $\mathbb{R}^4(i, j, k)$, the generator of $\pi_2(\mathfrak{Emb}_0(\mathbb{S}^1, \mathbb{S}^3))$ is the 2-sphere $\{\gamma_p : p \in \mathbb{S}^2(i, j, k)\}$, meaning that $\gamma_p(\theta) = \cos\theta + p \sin\theta$. It is clear that a normal framing for γ_i is given by $\tau_i(\theta) = \langle j, k\rangle$. We choose as equator the loop of curves γ_p with $p \in \mathbb{S}^1(j, k)$. We look for a family of diffeomorphisms $A_{p,r} : \mathbb{R}^4 \to \mathbb{R}^4$, $(p, r) \in \mathbb{S}^1(j, k) \times [0, 1]$, such that $A_{p,r}(\gamma_i) = \gamma_{(\cos\frac{\pi}{2}r)i + (\sin\frac{\pi}{2}r)p}$ and $A_{p,r}(1) = 1$. We can, indeed, choose $A_{p,r}$ to be the linear rotation of angle $\frac{\pi}{2}r$ around the axis defined by $\langle 1, i \cdot p\rangle$. With this choice it is clear that the $\mathbb{S}^1$-parametric family of knots $\gamma_p = A_{p,1}\gamma_i$ has an associated family of framings $\tau_p = \langle(\cos\phi)i + \sin\phi((\sin\phi)j - (\cos\phi)k), (\sin\phi)i + \cos\phi((\sin\phi)j - (\cos\phi)k)\rangle$, with $p = (\cos\phi)j + (\sin\phi)k$. Choosing the south pole $-i \in \mathbb{S}(i, j, k)$, we define the framing $\tau_{-i}(\theta) = \langle -j, -k\rangle$. We repeat the previous process but taking a family of linear isomorphisms preserving the axis $\langle 1, -i \cdot p\rangle$. Obviously, we get a $\mathbb{S}^1$-family of framings $\tilde{\tau}_p$ that satisfies $\tilde{\tau}_p = \tau_p$. We have proven that $d([\gamma_p]) = 0$.
- The connected component $\mathfrak{Emb}_{p,q}(\mathbb{S}^1, \mathbb{S}^3)$ of a non-trivial parametrized (p, q) torus knot has the homotopy type of SO(4) and the homotopy equivalence is induced by the action $\mathrm{Diff}^+(\mathbb{S}^3) \to \mathfrak{Emb}_{p,q}(\mathbb{S}^1, \mathbb{S}^3)$ (see [12], Theorem 1). Recall that $\mathrm{Diff}^+(\mathbb{S}^3)$ is homotopy equivalent to SO(4) (see [11]). In this case, $\mathrm{tb}_{\pi_1} \in \mathbb{Z}$ is always defined.

- The connected component $\mathfrak{Emb}'(\mathbb{S}^1, \mathbb{S}^3)$ of an hyperbolic parametrized knot γ has the homotopy type of $\mathbb{S}^1 \times \mathrm{SO}(4)$ (see [12], Theorem 1). In particular, $\mathfrak{Emb}'(\mathbb{S}^1, \mathbb{S}^3)$ has trivial second homotopy group. Moreover, the map $\pi_1(\Phi_\gamma)$ is injective. Thus, $\mathrm{tb}_{\pi_1} \in \mathbb{Z}$ is well defined for loops in $\mathrm{Image}(\Phi_\gamma)$ and for smoothly trivial loops.

20.4 The Formal Viewpoint

Following [9] we study Legendrians from a formal viewpoint in $(\mathbb{R}^3, \xi_{\mathrm{std}})$ and $(\mathbb{S}^3, \xi_{\mathrm{std}})$. The assumption of restricting to the standard structures is only made for simplicity in the statements.[1] For a more general discussion see [15].

20.4.1 Formal Legendrian Embeddings

Definition 9 Let (M, ξ) be $(\mathbb{R}^3, \xi_{\mathrm{std}})$ or $(\mathbb{S}^3, \xi_{\mathrm{std}})$. A *formal Legendrian embedding* into (M, ξ) is a pair (γ, F_s) such that

(i) $\gamma : \mathbb{S}^1 \to M$ is an embedding,
(ii) $F_s : \mathbb{S}^1 \to \gamma^*(TM \setminus \{0\})$, $s \in [0, 1]$, is a homotopy between $F_0 = \gamma'$ and $F_1 : \mathbb{S}^1 \to \gamma^*(\xi \setminus \{0\}) \subseteq \gamma^*(TM \setminus \{0\})$.

Trivialize TM and ξ. From now on we understand $F_s : \mathbb{S}^1 \to \mathbb{S}^2$ and $F_1 : \mathbb{S}^1 \to \mathbb{S}^1 = \mathbb{S}^2 \cap \xi$. On $(\mathbb{R}^3(x, y, z), \xi_{\mathrm{std}})$ we fix the framing $\xi_{\mathrm{std}} = \langle \partial_x + y\partial_z, \partial_y \rangle$. On $(\mathbb{S}^3, \xi_{\mathrm{std}})$ we fix the framing given by $\xi_{\mathrm{std}}(p) = \langle jp, kp \rangle$, where we are using quarternionic notation, i.e. $\mathbb{S}^3 \subseteq \mathbb{R}^4(i, j, k)$.

Denote by $\mathfrak{FLeg}(M, \xi)$ the space of formal Legendrian embeddings. In order to study the homotopy type of the space of formal Legendrians we introduce the following auxiliary space $\overline{\mathfrak{FLeg}}(M, \xi) = \mathfrak{Emb}(\mathbb{S}^1, M) \times L\mathbb{S}^1$, where LX denotes the free loop space of a connected manifold X. Recall that LX has the homotopy type of $X \rtimes \Omega_p(X)$ and, moreover, if X is a Lie group then $LX \cong X \times \Omega_1(X)$. We have a natural fibration

$$\begin{aligned} f : \mathfrak{FLeg}(M, \xi) &\longrightarrow \overline{\mathfrak{FLeg}}(M, \xi) \\ (\gamma, F_s) &\longmapsto \quad (\gamma, F_1). \end{aligned}$$

The morphism f is surjective. Indeed, given (γ, F_1) we need to find a homotopy between γ' and F_1 inside $L\mathbb{S}^2$. Since F_1 is null homotopic (in $L\mathbb{S}^2$) by the Legendrian condition, this is equivalent to say that γ' is null homotopic which is true, by dimensional reasons, for every embedding $\gamma \in \mathfrak{Emb}(\mathbb{S}^1, M)$. Fix as base point $(\gamma, \gamma') \in \overline{\mathfrak{FLeg}}(M, \xi)$, with $\gamma \in \mathfrak{Leg}(M, \xi)$. The fiber over this point

[1] In fact, the statements follow for any contact structure on $\mathbb{R}^3$ or $\mathbb{S}^3$.

is $\Omega_{\gamma'}(L\mathbb{S}^2)$. Denote the diagonal maps in the associated long exact sequence in homotopy by $\partial_k : \pi_k(\overline{\mathfrak{F}\mathfrak{Leg}}(M, \xi)) \to \pi_{k-1}(\Omega_{\gamma'}(L\mathbb{S}^2)) \cong \pi_k(L\mathbb{S}^2)$. Recall that, by the Smale-Hirsch h-principle for immersions [13], $\mathfrak{Imm}(\mathbb{S}^1, M)$ has the homotopy type of $LM \times L\mathbb{S}^2$. Let $p_2 : LM \times L\mathbb{S}^2 \to L\mathbb{S}^2$ be the projection onto the second factor and $i : \mathfrak{Emb}(\mathbb{S}^1, M) \hookrightarrow \mathfrak{Imm}(\mathbb{S}^1, M)$ the natural inclusion. We have the following.

Lemma 1 *The homorphisms ∂_k and $\pi_k(p_2) \circ \pi_k(i)$ coincide. More precisely, if $(\gamma^z, F_1^z) \in \pi_k(\overline{\mathfrak{F}\mathfrak{Leg}}(M, \xi))$ then*

$$\partial_k(\gamma^z, F_1^z) = \pi_k(p_2) \circ \pi_k(i)(\gamma^z) \in \pi_k(L\mathbb{S}^2).$$

Proof The image of (γ^z, F_1^z) by ∂_k measures the difference between the derivative $(\gamma^z)'$ and F_1^z as elements in $\pi_k(L\mathbb{S}^2)$. The homotopy class of F_1^z is zero by the Legendrian condition. Thus, $\partial_k(\gamma^z, F_1^z) = (\gamma^z)' \in \pi_k(L\mathbb{S}^2)$, i.e. $\partial_k(\gamma^z, F_1^z) = \pi_k(p_2) \circ \pi_k(i)(\gamma^z)$. □

With the previous discussion in mind one can conclude the following well known fact, we refer the reader to [9] or [15] for a proof.

Theorem 1 *Formal Legendrian embeddings are classified by their parametrized knot type, rotation number and Thurston–Bennequin invariant.*

About the fundamental group of the space of formal Legendrian embeddings we can state the following.

Theorem 2 ([9],Theorem 3.4.1) *Let $\gamma \in \mathfrak{Leg}(M, \xi)$ be a Legendrian embedding. Fix $(\gamma, \gamma') \in \mathfrak{F}\mathfrak{Leg}(M, \xi)$ as the base point. Then, there exist numbers $m_1, m_2 \in \mathbb{Z}_{\geq 0}$, depending only on the parametrized knot type of γ, such that the following sequence*

$$0 \longrightarrow \mathbb{Z}_{m_1} \oplus \mathbb{Z}_{m_2} \longrightarrow \pi_1(\mathfrak{F}\mathfrak{Leg}(M, \xi)) \longrightarrow \pi_1(\mathfrak{Emb}(\mathbb{S}^1, M)) \oplus \mathbb{Z} \longrightarrow 0$$

is exact. Moreover, the last $\mathbb{Z}$ factor corresponds to the Rot_{π_1} *invariant.*

20.5 The Action of $\mathrm{Cont}(\mathbb{S}^3, \xi_{\mathrm{std}})$ on the Space $\widehat{\mathfrak{Leg}}(\mathbb{S}^3, \xi_{\mathrm{std}})$

20.5.1 The Action of the Contactomorphism Group on the Space of Legendrians

Recall that on $\mathbb{S}^3 \subseteq \mathbb{C}^2$ the standard contact structure ξ_{std} is defined as the complex tangencies of the 3-sphere; i.e. $\xi_{\mathrm{std}}(p) = T_p\mathbb{S}^3 \cap i(T_p\mathbb{S}^3)$, $p \in \mathbb{S}^3$. Thus we have a natural inclusion

$$\mathrm{U}(2) \hookrightarrow \mathrm{Cont}(\mathbb{S}^3, \xi_{\mathrm{std}}). \tag{20.3}$$

This map has a geometrically left inverse given by the evaluation of the 1-jet of a contactomorphism at the north pole $N \in \mathbb{S}^3$. Hence, the last inclusion induces an injection in all homotopy groups. Moreover, it is a well known fact ([5]) that the inclusion $\mathrm{U}(2) \hookrightarrow \mathrm{Cont}(\mathbb{S}^3, \xi_{\mathrm{std}})$ is a weak homotopy equivalence (see [2] for a complete proof).

Consider the restriction of the natural action of the contactomorphism group on the space of Legendrians to the unitary group. Fix a Legendrian $L \in \widehat{\mathfrak{Leg}}(\mathbb{S}^3, \xi_{\mathrm{std}})$. The orbit of this Legendrian is described by the map

$$\begin{array}{rcl} \hat{\Phi}_L : \mathrm{U}(2) & \longrightarrow & \widehat{\mathfrak{Leg}}(\mathbb{S}^3, \xi_{\mathrm{std}}) \\ A & \longmapsto & A(L). \end{array} \tag{20.4}$$

Observe that we have an analogous action in the space of Legendrian embeddings. The orbit of $\gamma \in \mathfrak{Leg}(\mathbb{S}^3, \xi_{\mathrm{std}})$ is given by

$$\begin{array}{rcl} \Phi_\gamma : \mathrm{U}(2) & \longrightarrow & \mathfrak{Leg}(\mathbb{S}^3, \xi_{\mathrm{std}}) \\ A & \longmapsto & A \cdot \gamma. \end{array} \tag{20.5}$$

20.5.2 Homotopy Injection of $\mathbf{Cont}(\mathbb{S}^3, \xi_{\mathbf{std}})$ *in* $\widehat{\mathfrak{Leg}}(\mathbb{S}^3, \xi_{\mathbf{std}})$

The main result of this section is the following one.

Theorem 3 *The map*

$$\pi_k(\hat{\Phi}_L) : \pi_k(\mathrm{U}(2), \mathrm{Id}) \to \pi_k(\widehat{\mathfrak{Leg}}(\mathbb{S}^3, \xi_{\mathrm{std}}), L)$$

is an injection for all $k \geq 2$. Moreover, if one of the following conditions is satisfied

- $\mathrm{Rot}(L) = 0$ *or*
- $\mathrm{tb}(L) \neq 0$ *and L is an unknot or a torus knot or a hyperbolic knot,*

then the map $\pi_1(\hat{\Phi}_L)$ is also an injection.

Remark 3 By Proposition 1 the second condition is always satisfied for any Legendrian unknot. Moreover, the classification of the Legendrian figure eight knots (see [8]) implies that the second condition is always satisfied.

Proof For $p \in \mathbb{S}^3$, we have that $\xi_{\mathrm{std}}(p) = \langle jp, kp \rangle$. Let $\gamma \in \mathfrak{Leg}(\mathbb{S}^3, \xi_{\mathrm{std}})$ be any parametrization of L. Since the unitary groups acts transitively on $\mathbb{S}^3$ we may assume that $\gamma(0) = (1, 0)^t \in \mathbb{S}^3 \subseteq \mathbb{C}^2$. □

Lemma 2 *The maps*

$$\pi_k(\Phi_\gamma) : \pi_k(\mathrm{U}(2), \mathrm{Id}) \to \pi_k(\mathfrak{Leg}(\mathbb{S}^3, \xi_{\mathrm{std}}), \gamma)$$

are injective for all k.

Proof The composition

$$\begin{array}{ccccc} \mathrm{SU}(2) & \longrightarrow & \mathfrak{Leg}(\mathbb{S}^3, \xi_{\mathrm{std}}) & \longrightarrow & \mathbb{S}^3 \\ A & \longmapsto & A \cdot \gamma & \longmapsto & A(\gamma(0)), \end{array}$$

defines a diffeomorphism. Thus, since $\pi_k(\mathrm{U}(2)) \cong \pi_k(\mathrm{SU}(2))$ for $k \geq 2$, we conclude that $\pi_k(\Phi_\gamma)$ is injective for $k \geq 2$.

Observe that $\pi_1(\mathrm{U}(2)) = \{[A_\theta]^m = [A_\theta^m] : m \in \mathbb{Z}\}$ where

$$A_\theta = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix}, \theta \in \mathbb{S}^1.$$

Hence,

$$\mathrm{Rot}_{\pi_1}(A_\theta^m \cdot \gamma) = m$$

and $\pi_1(\Phi_\gamma)$ is also injective. □

Since $\widehat{\mathfrak{Leg}}(\mathbb{S}^3, \xi_{\mathrm{std}}) = \mathfrak{Leg}(\mathbb{S}^3, \xi_{\mathrm{std}})/\mathrm{Diff}^+(\mathbb{S}^1)$ the last lemma implies that $\pi_k(\hat{\Phi}_L)$ is injective for $k \geq 2$.

To conclude the injectivity of the map $\pi_1(\hat{\Phi}_L)$ we must check that the loops $A_\theta^m(L)$, $m \neq 0$, are non trivial for any choice of parametrization. The possible parametrizations of these loops are given by

$$\gamma_m^{\theta,k}(t) = A_\theta^m \gamma(t - k\theta), k \in \mathbb{Z}.$$

Assume that there exists $k \in \mathbb{Z}$ such that $\gamma_m^{\theta,k}$ is trivial. Thus,

$$\mathrm{Rot}_{\pi_1}(\gamma_m^{\theta,k}) = \mathrm{Rot}_{\pi_1}(\gamma_m^{\theta,0}) - k\,\mathrm{Rot}(L) = m - k\,\mathrm{Rot}(L) = 0. \tag{20.6}$$

Hence, if $\mathrm{Rot}(L) = 0$ the map $\pi_1(\hat{\Phi}_L)$ is injective.

From now on assume that L is an unknot or a torus knot or a hyperbolic knot. The tb_{π_1} invariant is always well defined for the unknot and any torus knot. Moreover, for a hyperbolic knot tb_{π_1} is well defined in $\mathrm{Image}(\hat{\Phi}_L)$. Assume that there exists $k \in \mathbb{Z}$ such that $\gamma_m^{\theta,k}$ is trivial for $m \neq 0$. Thus, $k \neq 0$ by (20.6). On the other hand

$$\mathrm{tb}_{\pi_1}(\gamma_m^{\theta,k}) = \mathrm{tb}_{\pi_1}(\gamma_m^{\theta,0}) - k\,\mathrm{tb}(L) = -k\,\mathrm{tb}(L) = 0. \tag{20.7}$$

Realize that, since $\gamma_m^{\theta,0} = A_\theta^m \cdot \gamma^0$. Thus, after fixing a Seifert surface S_0 for γ^0, we get a family of Seifert surfaces S_θ and it is clear that $\mathrm{tb}_{\pi_1}(\gamma_m^{\theta,0}) = 0$. Hence, if $\mathrm{tb}(L) \neq 0$ the map $\pi_1(\hat{\Phi}_L)$ is an injection. □

20.5.3 Non Injectivity of the Map $\pi_1(\widehat{\mathfrak{Leg}}(\mathbb{S}^3, \xi_{\mathrm{std}}), L) \to \pi_1(\widehat{\mathcal{K}}(\mathbb{S}^3), L)$

Let $\widehat{\mathcal{K}}(\mathbb{S}^3)$ be the space of embedded circles in $\mathbb{S}^3$. The map (20.4) allows us to construct plenty of examples of loops which are homotopically trivial in the smooth category, i.e. inside $\widehat{\mathcal{K}}(\mathbb{S}^3)$, but non-trivial in the Legendrian setting.

Proposition 4 *Let $L \in \widehat{\mathfrak{Leg}}(\mathbb{S}^3, \xi_{\mathrm{std}})$ be a Legendrian which satisfies one of the following conditions:*

- $|\mathrm{Rot}(L)| \neq 1, 2$ *or*
- $\mathrm{tb}(L) \neq 0$ *and L is an unknot or a torus knot or a hyperbolic knot.*

Then, the homomorphism $\pi_1(\widehat{\mathfrak{Leg}}(\mathbb{S}^3, \xi_{\mathrm{std}}), L) \to \pi_1(\widehat{\mathcal{K}}(\mathbb{S}^3), L)$, induced by the inclusion, is non injective.

Proof Assume that the second condition holds. Let $m \neq 0$ be any even integer, by Theorem 3 the loop $A_\theta^m(L)$ is non-trivial. Finally, observe that since m is even A_θ^m is trivial as a loop in $\mathrm{SO}(4)$. Thus, $A_\theta^m(L)$ is homotopically trivial inside $\widehat{\mathcal{K}}(\mathbb{S}^3)$.

On the other hand, assume that the first condition holds. Let $\gamma \in \mathfrak{Leg}(\mathbb{S}^3, \xi_{\mathrm{std}})$ be any parametrization of L. Take $m = \mathrm{Rot}(L) + 2$ if $\mathrm{Rot}(L)$ is even and $m = \mathrm{Rot}(L) + 1$

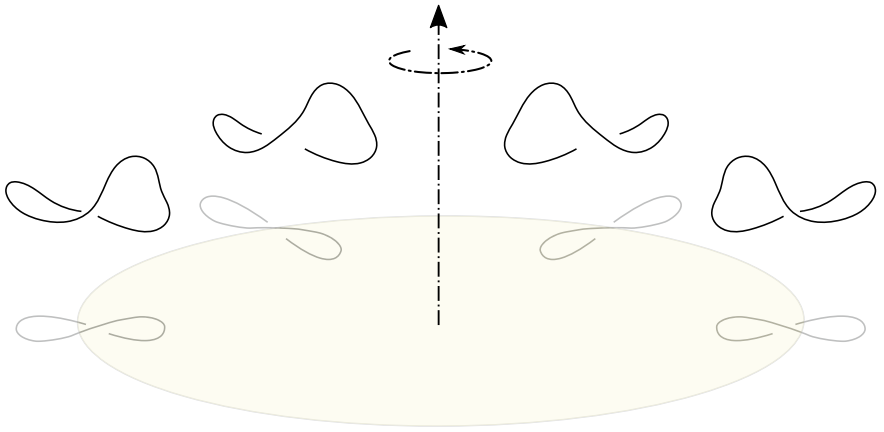

Fig. 20.1 Schematic picture of the loop $A_\theta^m(L)$ for the standard Legendrian unknot L, $\theta \in [0, \pi/m]$

if it is odd. Since m is even $A_\theta^m(L)$ is trivial in $\widehat{\mathcal{K}}(\mathbb{S}^3)$. However, the loop $A_\theta^m(L)$ is non-trivial inside $\widehat{\mathfrak{Leg}}(\mathbb{S}^3, \xi_{\text{std}})$. Indeed, all the parametrizations of the loop are given by $\gamma_m^{\theta,k}(t) = A_\theta^m \gamma(t - k\theta)$. The equality $\text{Rot}_{\pi_1}(\gamma_m^{\theta,k}) = m - k\,\text{Rot}(L) = 0$ cannot hold for any $k \in \mathbb{Z}$ since it implies that $\text{Rot}(L)$ divides 1 or 2 and this is not true (Fig. 20.1). □

Acknowledgements We want to specially thank Alberto Ibort for his support of our research in the last few years. In particular he has been an excellent listener of the study of the topology of the spaces of horizontal embeddings, of which the Legendrian spaces are particular instances.
The authors are supported by the Spanish Research Projects SEV–2015–0554, MTM2016–79400–P, and MTM2015–72876–EXP. The first author is supported by a Beca de Personal Investigador en Formación UCM. The second author is funded by Programa Predoctoral de Formación de Personal Investigador No Doctor del Departamento de Educación del Gobierno Vasco.

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G. Marmo et al. (eds.), *Classical and Quantum Physics*,
Springer Proceedings in Physics 229,
https://doi.org/10.1007/978-3-030-24748-5